Bridging Scale and Domain Reduction Approaches to Multiscale Computations

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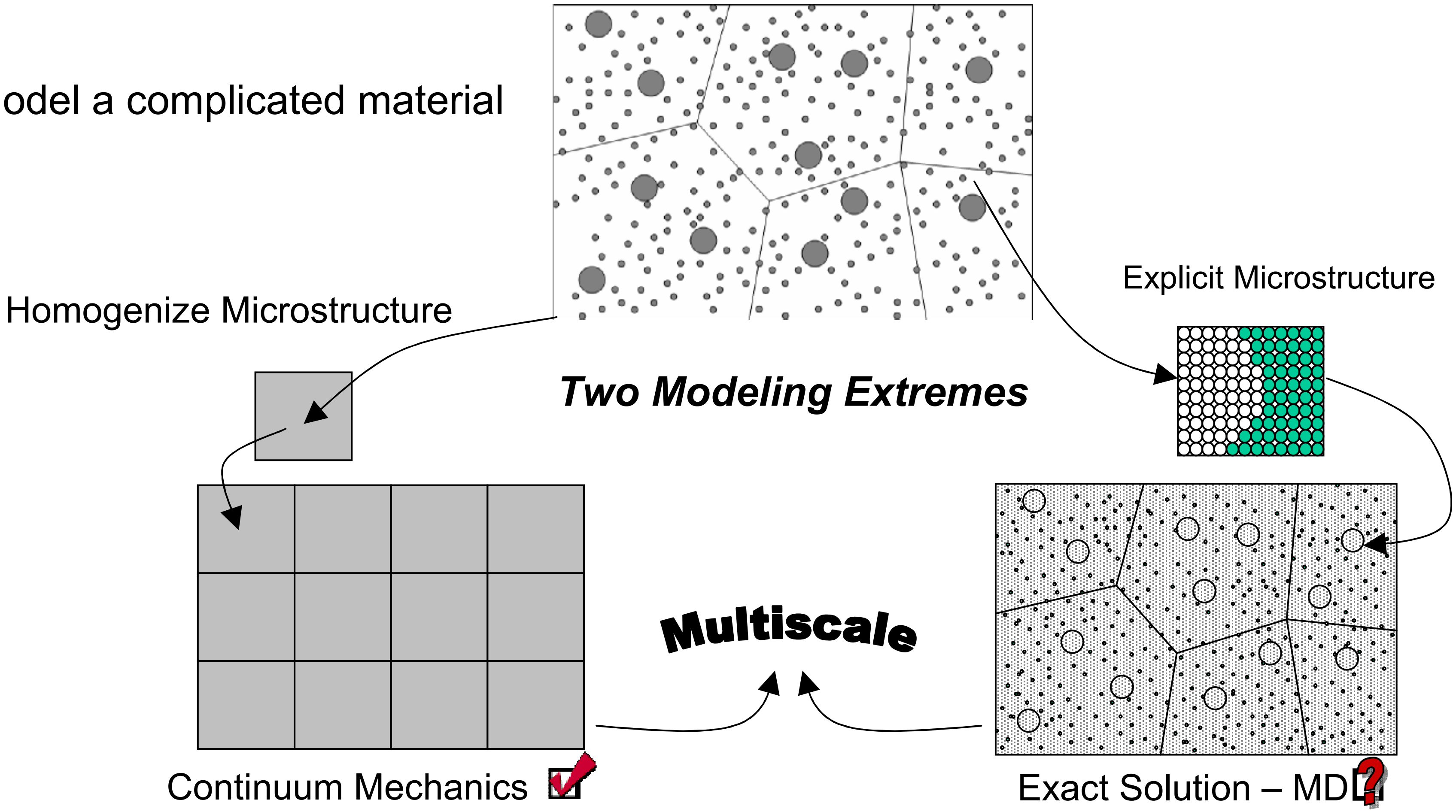
Motivation

Model a complicated material



Two types of coupling approaches:

- Interfacial AtC + Quantum Effects
- Homogenization theories

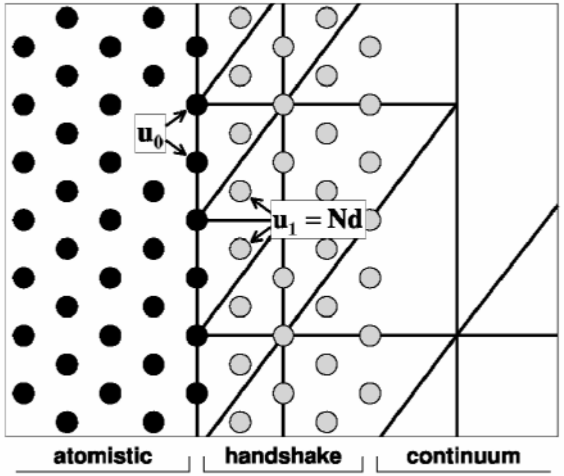
Plan

- **Typical issues of hybrid multiscale modelling**
- **Bridging Scale method with application to fracture**
- **Multiscale Boundary Condition (domain reduction) approach with application to nanoindentation**
- **Virtual Atom Cluster (coupling with ab initio) approach**
- **Multiresolution continuum framework**

Typical Issues

1. True coarse scale discretization
2. Interfacial wave reflection
3. Double counting of the strain energy
4. Implementation: usage of existing MD and continuum codes; parallel computing
5. Dynamic mesh refinement/enrichment
6. Finite temperatures
7. Quantum-mechanical effects (Electron-mechanical coupling)
8. Multiple scales for continua
9. Multiple time scales and dynamics of infrequent events

Typical interface model

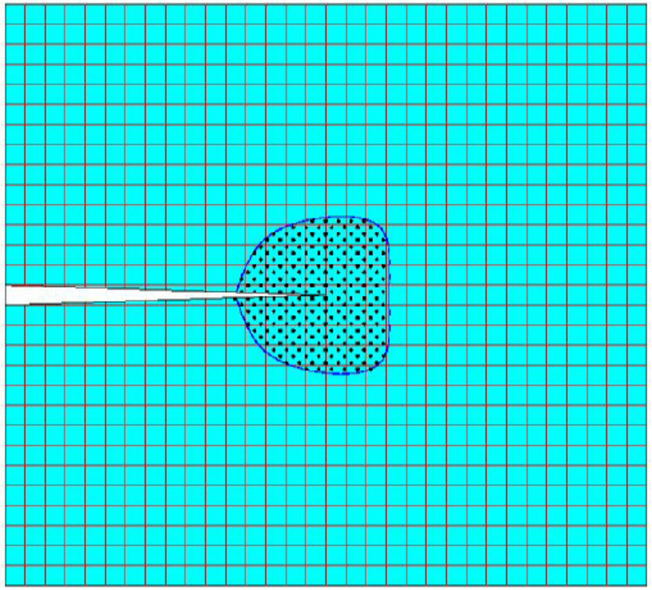


- BSM addresses issues 1-2, and partially 3-6.
- MSBC method: issues 1-4 DO NOT ARISE
- Virtual Atom Cluster method – deals with 7
- Multiresolution Continuum Approach – deals with 8

The Bridging Scale Method

- **Two most important components:**
  - bridging scale projection
  - impedance boundary conditions applied MD/FE interface in the form of a time-history integral

- Assumes a *single* solution $\mathbf{u}(x)$ for the *entire domain*. This solution is *decomposed into the fine and coarse scale fields:*



$$\mathbf{u}(x) = \bar{\mathbf{u}}(x) + \mathbf{u}'(x)$$

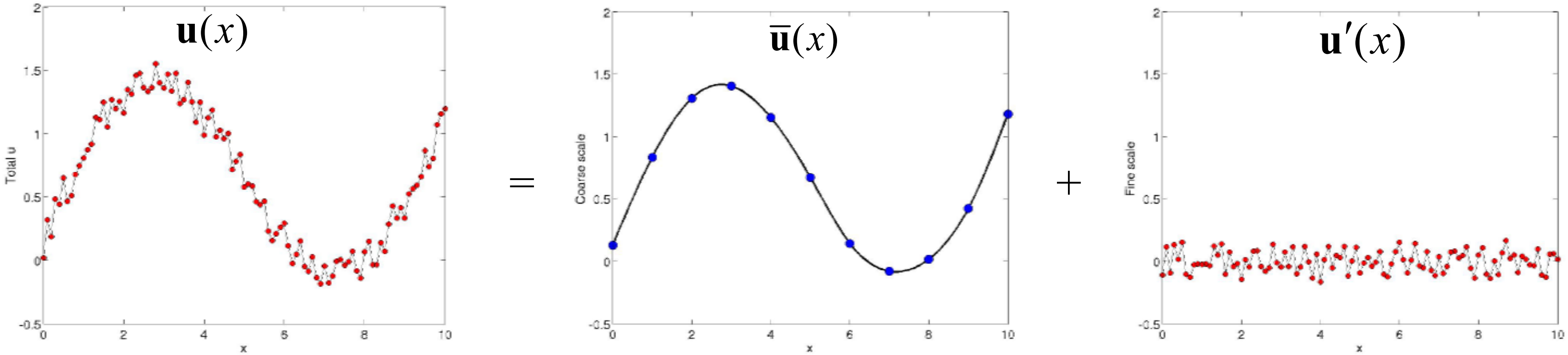
BS projection

$$\bar{\mathbf{u}}(x) = \mathbf{P}\mathbf{u}(x)$$

$$\mathbf{u}'(x) = \mathbf{u}(x) - \mathbf{P}\mathbf{u}(x) = (\mathbf{I} - \mathbf{P})\mathbf{u}(x) = \mathbf{Q}\mathbf{u}(x)$$

$$\mathbf{M} = \mathbf{N}^{\mathrm{T}}\mathbf{M}_A\mathbf{N}$$

$$\mathbf{Q} = \mathbf{I} - \mathbf{N}\mathbf{M}^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{M}_A$$



Multiscale Lagrangian

$$L = (\mathbf{d}, \dot{\mathbf{d}}, \mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{d}}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{d}} + \frac{1}{2}\dot{\mathbf{q}}^{\mathrm{T}}\left(\mathbf{Q}^{\mathrm{T}}\mathbf{M}_A\right)\dot{\mathbf{q}} - U(\mathbf{d}, \mathbf{q})$$

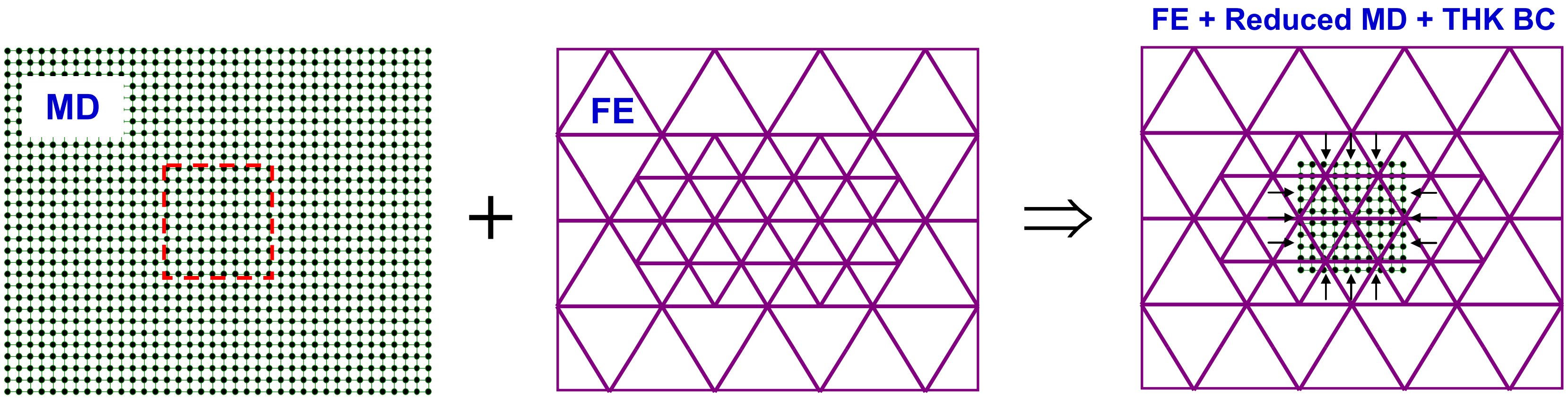
Lagrangian formulation gives coupled, coarse and fine scale, **equations of motion**

$$\boxed{\begin{aligned} \mathbf{M}\ddot{\mathbf{d}} &= \mathbf{N}^{\mathrm{T}}\mathbf{f}(\mathbf{u}) \\ \mathbf{M}_A\ddot{\mathbf{q}} &= \mathbf{Q}^{\mathrm{T}}\mathbf{f}(\mathbf{u}) \end{aligned} \qquad \mathbf{f} = \frac{\partial U}{\partial \mathbf{u}}}$$

The MD domain is too large to solve, so that we *eliminate* the MD degrees of freedom outside the localized domain of interest. Collective atomic behavior of in the bulk material is represented by an **impedance (THK) force** applied at the formal MD/continuum interface:

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{d}} &= \mathbf{N}^{\mathrm{T}}\mathbf{f}(\mathbf{u}) \\ \mathbf{M}_A\ddot{\mathbf{q}} &= \mathbf{f}(\mathbf{u}) + \boxed{\int_0^t \boldsymbol{\Theta}(t-\tau)\left(\mathbf{q}(\tau) - \bar{\mathbf{u}}(\tau)\right)d\tau + \mathbf{R}(t)} \end{aligned} \Rightarrow$$

Peripheral MD degrees of freedom are represented implicitly

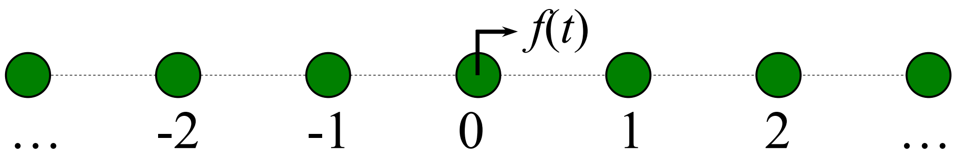


Wagner, Liu, 2003

Karpov, Wagner, Liu, 2004

Time History Kernel (THK)

The **time history kernel** shows the dependence of dynamics *in two adjacent cells*. Any time history kernel is related to the response function.



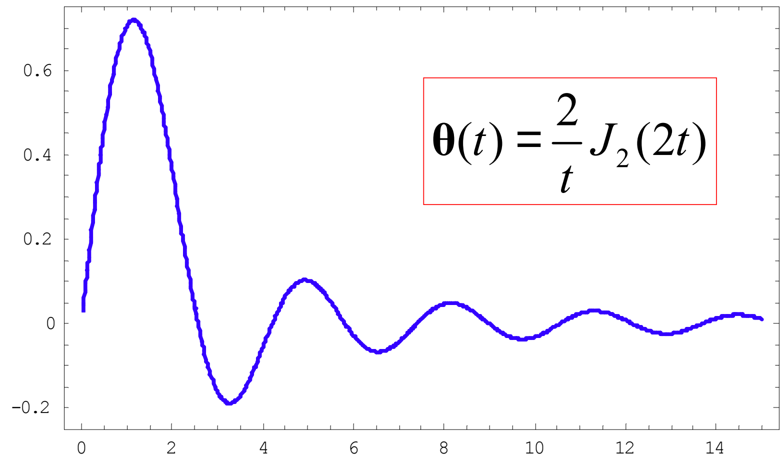
$$\mathbf{u}_1(t) = \Theta\{\mathbf{u}_0(t)\}, \quad \Theta = ?$$

$$\mathbf{f}_n(t) = \delta_{n,0}\mathbf{f}(t)$$

$$\mathbf{u}_n(t) = \int_0^t \mathbf{g}_{n-n'}(t-\tau) f(\tau)d\tau, \quad \mathbf{U}_n(s) = \mathbf{G}_n(s)\mathbf{F}(s), \quad \mathbf{U}_1(s) = \mathbf{G}_1(s)\mathbf{G}_0^{-1}(s)\mathbf{U}_0(s)$$

$$\boxed{\mathbf{u}_1(t) = \int_0^t \Theta(t-\tau)\mathbf{u}_0(\tau)d\tau, \quad \Theta(t) = \mathcal{L}^{-1}\left\{\mathbf{G}_1(s)\mathbf{G}_0^{-1}(s)\right\}}$$

$$\Theta(t) = \mathcal{L}^{-1}\left\{\frac{1}{4}\left(\sqrt{s^2+4} - s\right)^2\right\} = \frac{2}{t}J_2(2t)$$



Karpov EG, Wagner GJ, Liu WK. *IJNME* 62(9), 1250-1262, 2005.

Numerical Laplace Transform Inversion

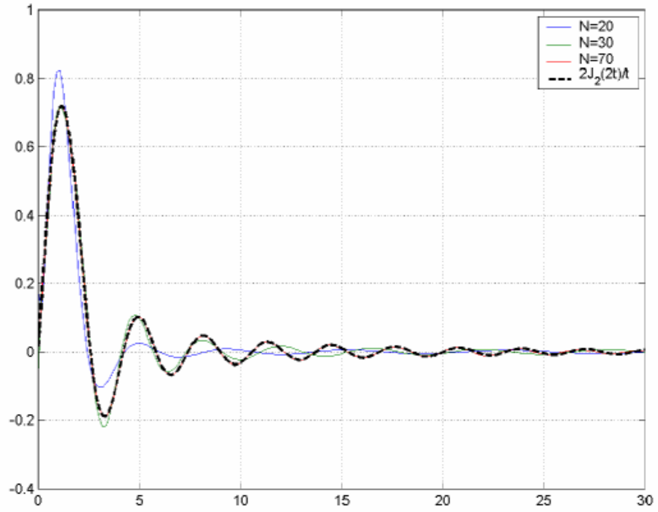
Most numerical algorithms for the Laplace transform inversion utilize series decompositions of the sought originals $f(t)$ in terms of functions whose Laplace transform is known. The expansion coefficients are found numerically from $F(s)$.

Examples:

- **Weeks algorithm**
  (*J Assoc Comp Machinery* 13, 1966, p.419)

$$f\left(t\right) \approx e^{\left(c-T/2\right)t} \sum_{\gamma=0}^{S} a_\gamma L_\gamma \left(t/T\right)$$

$L_\gamma(t)$ – Laguerre polynomials,
a_γ – coefficients computed using $F(s)$

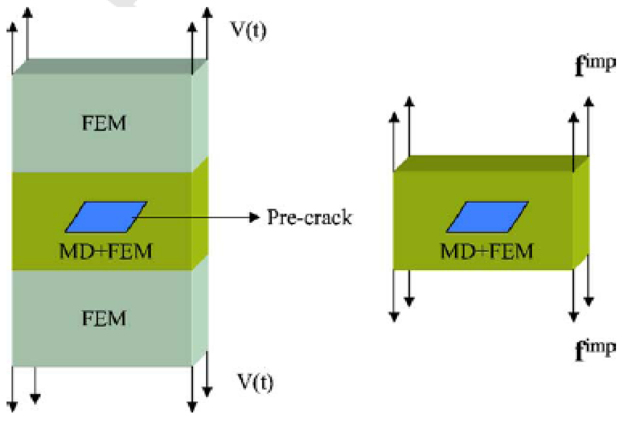


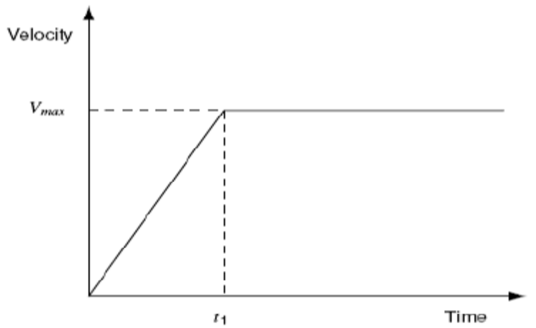
- **Sin-series expansion (*J Assoc Comp Machinery* 23, 1976, p.89)**
  For an odd function f gives

$$f\left(t\right) \approx -2\sum_{k=1}^{N} \operatorname{Im} F\left(\frac{k\pi i}{T}\right) \sin\left(\frac{k\pi t}{T}\right)$$

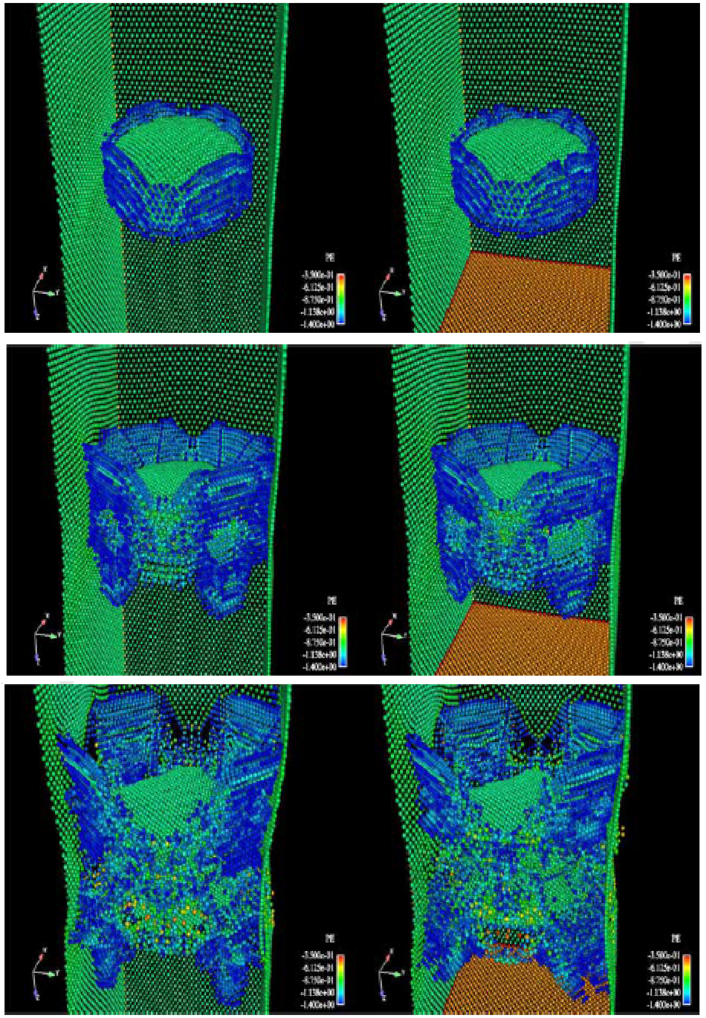
Problem description and comparison with the benchmark (full atomistic) solution

Problem description





Snapshots Comparison



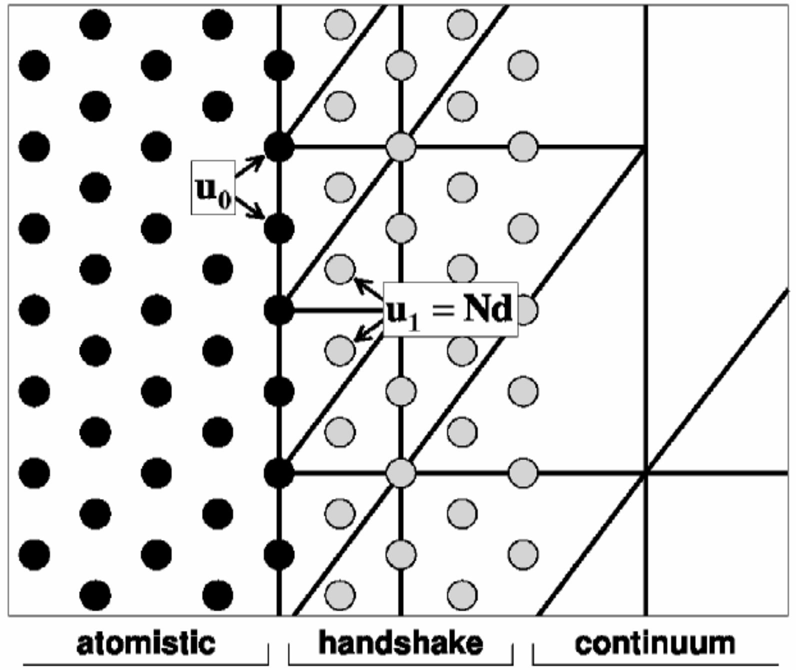
Results are identical; all features of the atomistic process are reproduced by the bridging scale model

Park HS, Karpov EG, Klein PA, Liu WK, Three-Dimensional Bridging Scale Analysis of Dynamic Fracture. *JCP* 207, 588-609, 2005.

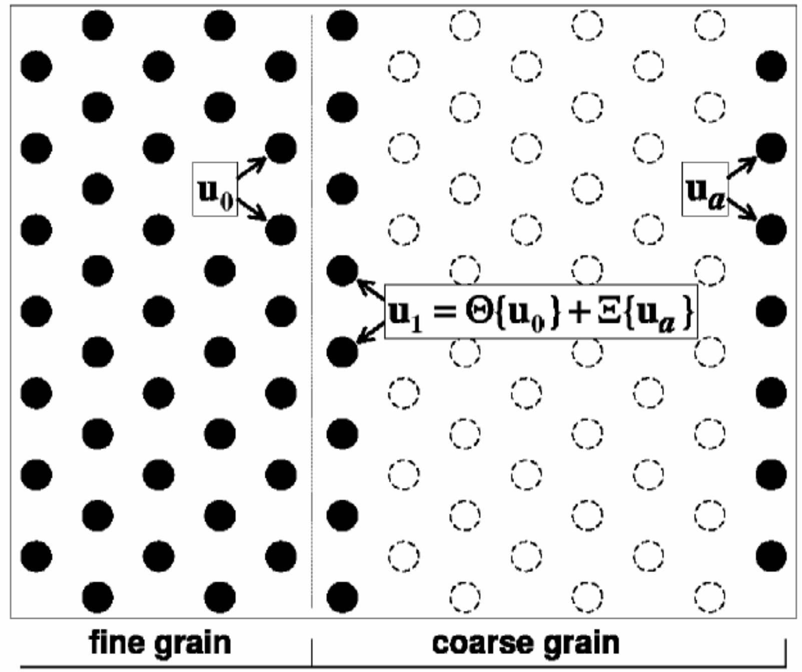
Multiscale Boundary Conditions (MSBC)

All excitations propagate with "infinite" velocities in the quasistatic case.
Provided that effect of peripheral boundary conditions, $\mathbf{u}_a$, is taken into account by lattice methods, the continuum model can be omitted

Standard hybrid method

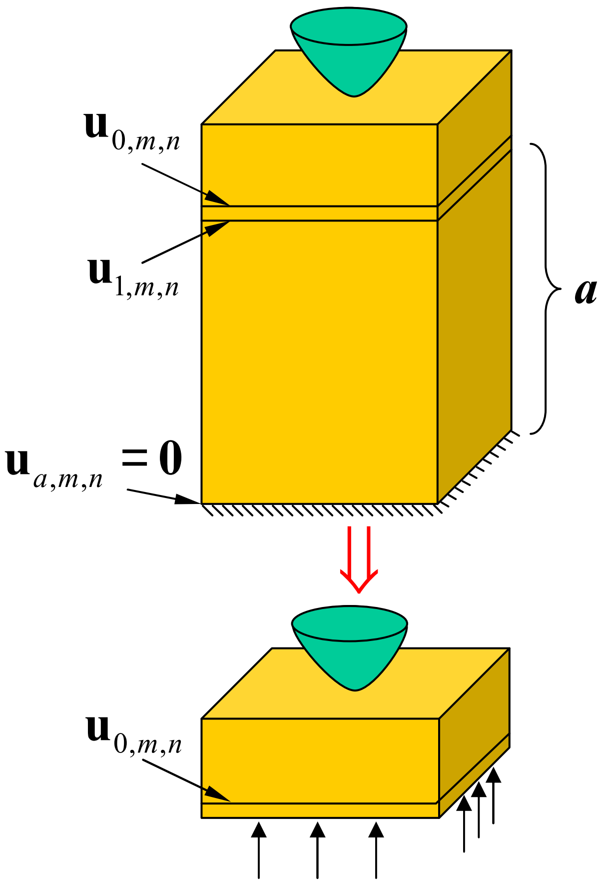


Multiscale boundary conditions



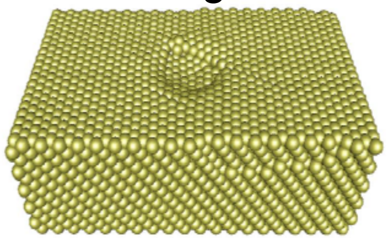
The MSBC involve no handshake domain with "ghost" atoms. Positions of the interface atoms are computed based on the **boundary condition operators Θ and Ξ**. The issue of double counting of the potential energy within the handshake domain does not arise.

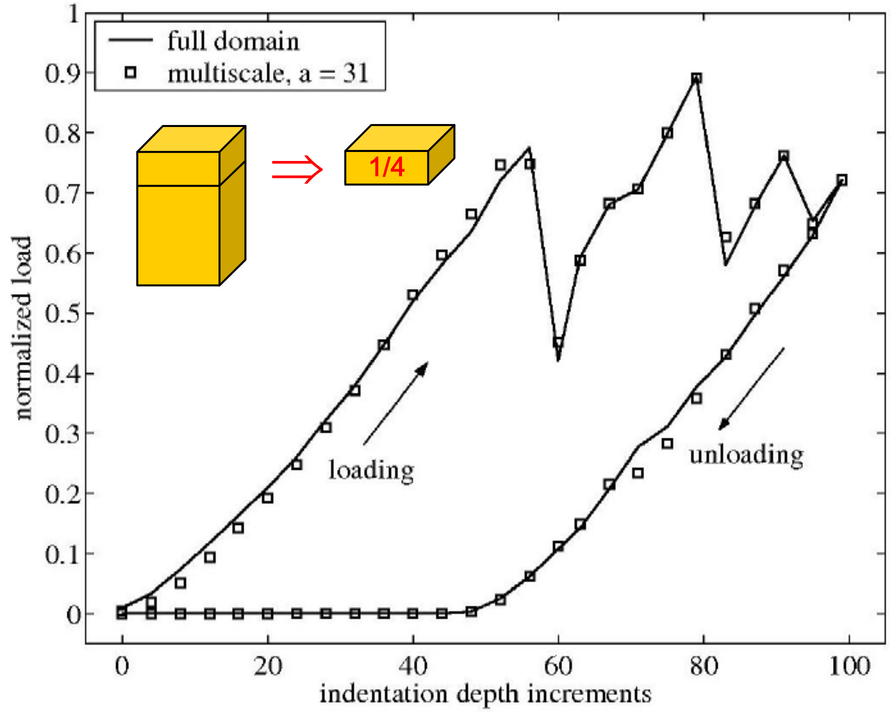
Nanoindentation: Domain Reduction



$$\boxed{\mathbf{u}_{1,m,n} = \sum_{m',n'} \mathbf{\Theta}^{(a)}_{m-m',n-n'} \mathbf{u}_{0,m',n'}}$$

FCC gold



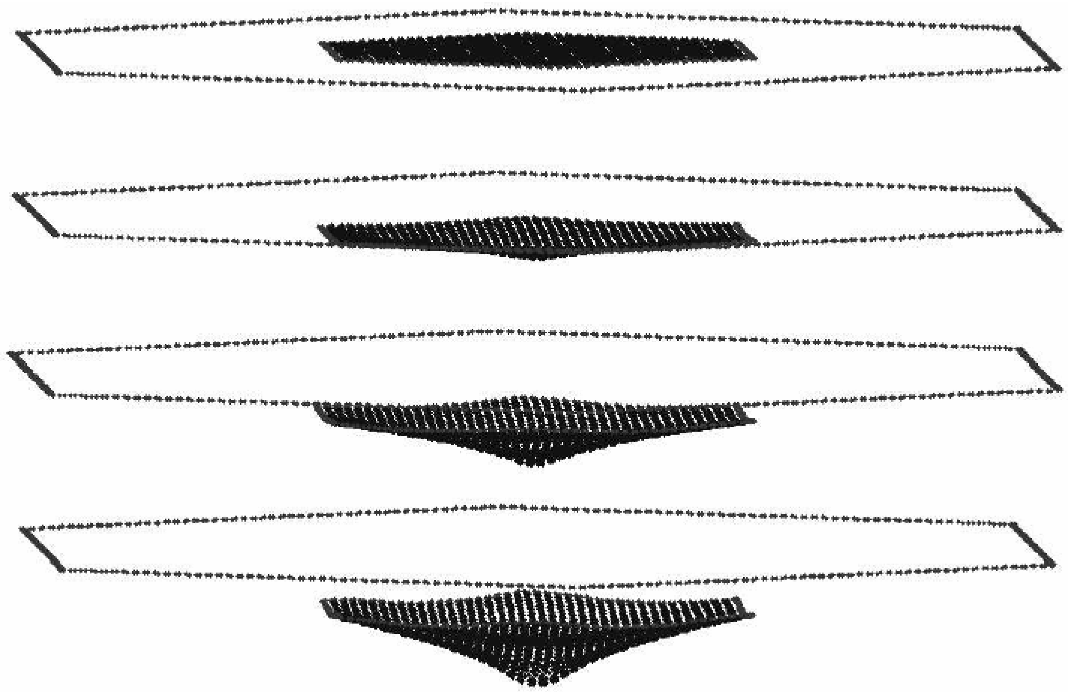


Karpov EG, Yu H, Park HS, Liu WK, Wang JQ, Qian D. Multiscale Boundary Conditions in Crystalline Solids: Theory and Application to Nanoindentation, *IJSS.* Available on-line.

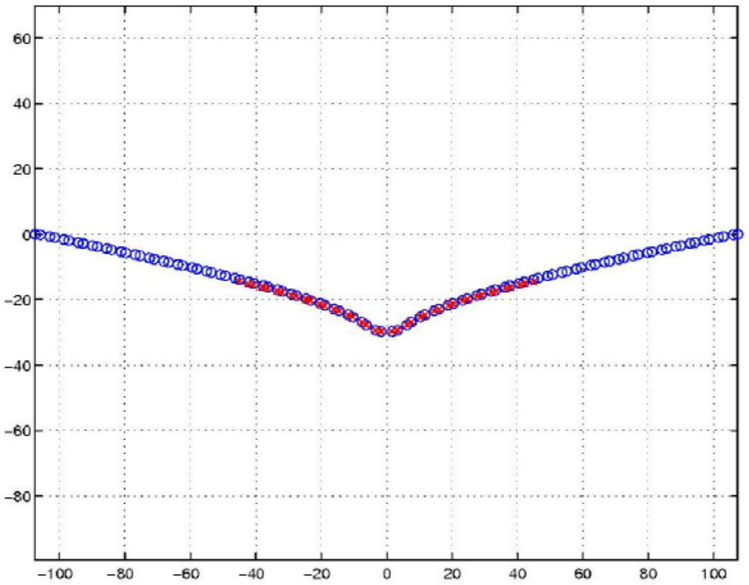
MSBC: Deformation of Graphene Monolayers

Shown is the reduced domain simulations with MSBC parameter a=10; the **true aspect ration** image (non-exaggerated). Error is still less than 3%. Tersoff-Brenner potential.

Deformation



Comparison
(red – MSBC, blue – benchmark)



Shown: vertical displacements of the atoms

Medyanik SN, Karpov EG, Liu WK. Domain Reduction Approach to Molecular Mechanics Simulations of Carbon Nanostructures. *Journal Computational Physics. 2006.* Accepted.

Discussion on the MSBC

Attractive features of the MSBC:

- SIMPLICITY
- no handshake issues (strain energy, interfacial mesh)
- in many applications, continuum model is not required
- performance does not depend on the size of coarse scale domain
- implementation for an available MD code is easy

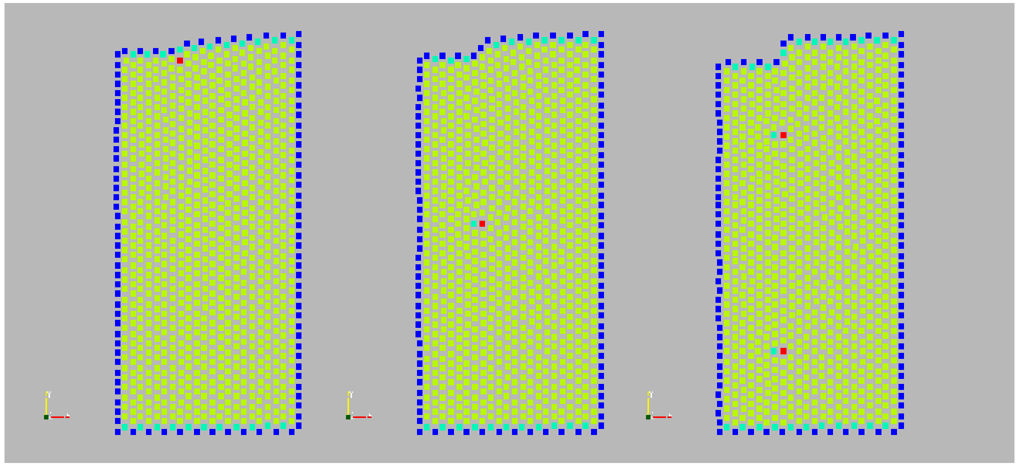
Limitations:

- simple geometries only

Perspectives:

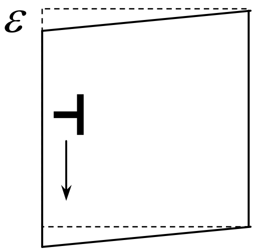
- passage of dislocations through the interface
- dynamic extension

Due to high mobility, lattice dislocations may reach the atomistic continuum interface before the simulation is complete.



Estimate:

$$v = \frac{\dot{\varepsilon}}{b\rho}$$



$\rho = 10^{-3}\,\text{ang}^{-2}, \quad \dot{\varepsilon} = 0.02\,\text{ps}^{-1},$

$b = 2\,\text{ang} \quad \Rightarrow \quad v \sim 10\,\text{ang/ps}$

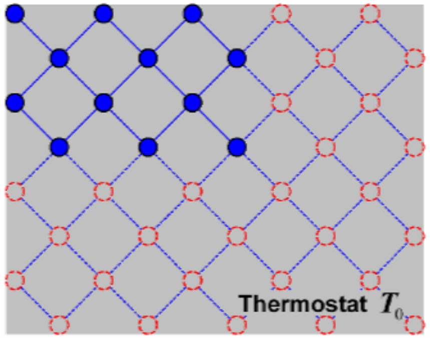
Passage of the dislocations through the interface:

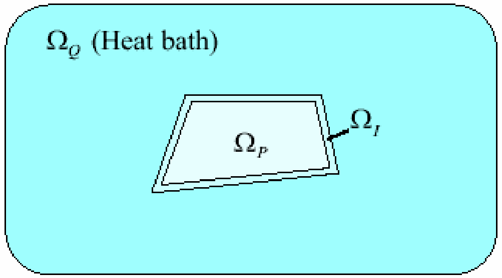
$$u = u^{df} + u^{d}, \quad u^{d} = Pu \quad \Rightarrow$$

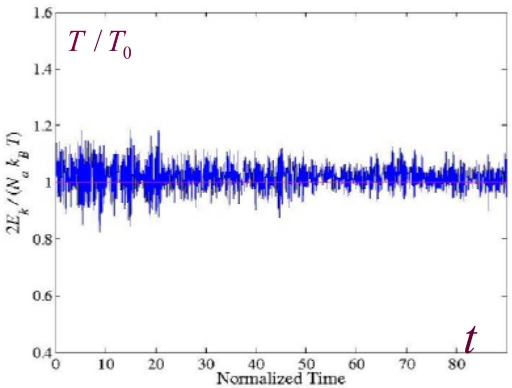
$$\mathbf{u}_1(t) = \int_0^t \Theta(t-\tau)\big(\mathbf{u}_0(\tau) - \mathbf{P}\mathbf{u}_0(\tau)\big)\,d\tau + \mathbf{u}_1^d(t)$$

Finite Temperatures: Phonon Heat Bath

Phonon heat bath represents energy exchange due to correlated motion of lattice atoms along the atomistic/continuum (solid-solid) interface







Process of heat exchange is correlated in time and space, therefore,

$$m\ddot{\mathbf{u}}_n(t) = -\frac{\partial U\left(\mathbf{u}^P, \mathbf{u}^I, \mathbf{u}^Q\right)}{\partial \mathbf{u}_n},$$

$$\mathbf{u}_n^Q = \sum_{n'} \int_0^t \Theta_{n-n'}(t-\tau)\left(\mathbf{u}_{n'}^I(\tau) - \mathbf{R}_{n'}^I(\tau)\right) d\tau + \mathbf{R}_n^Q(t)$$

$\Theta(t)$ – mechanical response of the thermostat

$\mathbf{R}(t)$ – random thermal fluctuations of thermostat atoms

Generally:

$$\boxed{\mathbf{R}_n(t) = \mathbf{M}\sum_{n'}\left(\mathbf{g}_{n-n'}(t)\,\dot{\mathbf{u}}_{n'}(0) + \dot{\mathbf{g}}_{n-n'}(t)\,\mathbf{u}_{n'}(0)\right)}$$

Alternatively:

$$\boxed{\mathbf{R}(t) = \sum_p a_p \mathbf{d}_p \sin(\omega_p t + \varphi_{p,n})}$$

$a_p(T_0)$ – sampled from the Gibbs distribution

Karpov EG, Park HS, Liu WK. A Phonon Heat Bath for Atomistic and Multiscale Simulation of Solids. Submitted.

Discussion: Autocorrelation of Thermal Fluctuations

$\mathbf{R}(t)$ is a complex random process.

Is it possible to handle $\mathbf{R}(t)$ in an averaged sense?

Other representations, besides the normal modes?

Can be shown generally:

$$\left\langle \dot{\mathbf{R}}_n(t) \right\rangle = \mathbf{0}$$

(can be extended also for the random force)

$$\left\langle \dot{\mathbf{R}}_n(t'+t)\dot{\mathbf{R}}_{n'}(t') \right\rangle = k_B T \, \underline{\dot{\mathbf{g}}_{n-n'}(t)}$$

... (higher order correlations) ...

Then

$$\boxed{\left\langle \dot{\mathbf{R}}_n(t) \right\rangle, \ \left\langle \dot{\mathbf{R}}_n(t'+t)\dot{\mathbf{R}}_{n'}(t') \right\rangle \quad \rightarrow \quad \mathbf{R}_n(t)}$$

However, solution to this problem is not unique.

- Is it possible that all higher order momentum are trivial?
- Any solution $\mathbf{R}(t)$ is acceptable; energy arguments?
- If not: What other conditions apply to $\mathbf{R}(t)$ (besides the correlation rules)?

Discussion on the Bridging Scale Method

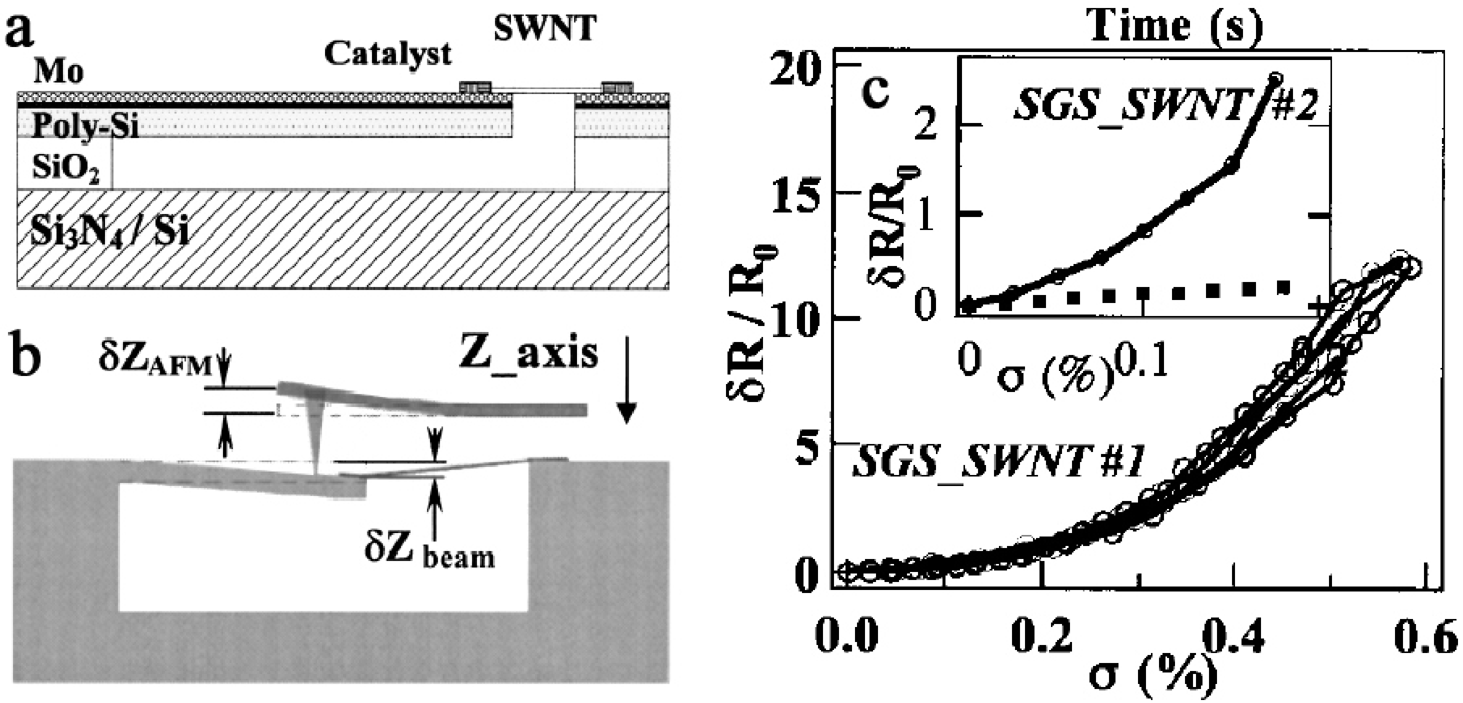
Attractive features of the BSM:

- bridging scale projection ⇨ true separation of scales
- time-history integral ⇨ no wave reflection
- implementation for available MD and FEM codes is easy

Current work and perspectives:

- Passage of dislocations through the interface
- Finite temperatures
- Electron-mechanical coupling effects (details to follow)
- Multiresolution continuum approach (details to follow)

Quantum-mechanical coupling phenomenon: Electron-Mechanical Interactions in Nanomaterials



(a) A schematic showing the device structure for the near-tensile testing of a suspended single walled CNT; (b) A schematic showing the principle of inducing tensile stretching in CNT by the deflection of the cantilever; (c) The measured resistance change versus strain curve. (Cao, Wang and Dai, PRL, 2003)

Motivation for Coupled Electron-Mechanical Analysis

- The Structures of the Electrons determines:
  - The structure of the molecule (bond length, angle)
  - Thermal properties (Electron-phonon interaction)
  - Electrical properties (conductance, polarizability)
  - Chemical reactivities (bond order, reaction barrier)
  - Mechanical properties (Stiffness, strength)

- The classical atomistic simulation methods based on empirical potentials do not provide direct information on the electronic structures.

- First-principle methods can fully resolve these interactions, but are limited in both the length and time scales it can handle.

Need for multiscale multiphysics modeling approach

Modeling and Simulation at Atomic scale

Schrödinger equation

Born-Oppenheimer Approximation

"Simplified" Schrödinger equation

"*ab initio*" Method (Hatree-Fock Approximation, Density Functional Theory, Tight-binding method…)

"*ab initio*" Molecular Dynamics

Inter-atomic interaction and electronic Wave function are fully coupled

Empirical Potential used in MD

Inter-atomic interaction is expressed in Certain empirical functional form and Decoupled from the wave function

Development of Multiscale Method

- Hierarchical Approach

  Coarse scale model rigorous derived from the atomistic model (e.g. hyperelastic theory)

  Can not fully resolve fine scale features such as defects, dislocation.

  Simulation of finite temperature problems currently being studied.

  A coarse grained model that directly incorporates the electronic descriptions is NOT yet available

- Concurrent approach

  Examples include the QC method, CADD, BSM, multiscale projection method, and bridge domain method…….

  Multiscale Interface is an important topic

  Most of the existing models focus only on the mechanical aspect.

A Quantum-mechanical-based Hierarchical Model : Tasks

- Mechanical aspect
  - The inter-atomic interaction resolved from first-principle method must be passed on to a coarse scale simulation technique such as finite element methods through a robust constitutive model
  - The degrees of freedom at atomic scale and at the coarse scale must be consistently linked

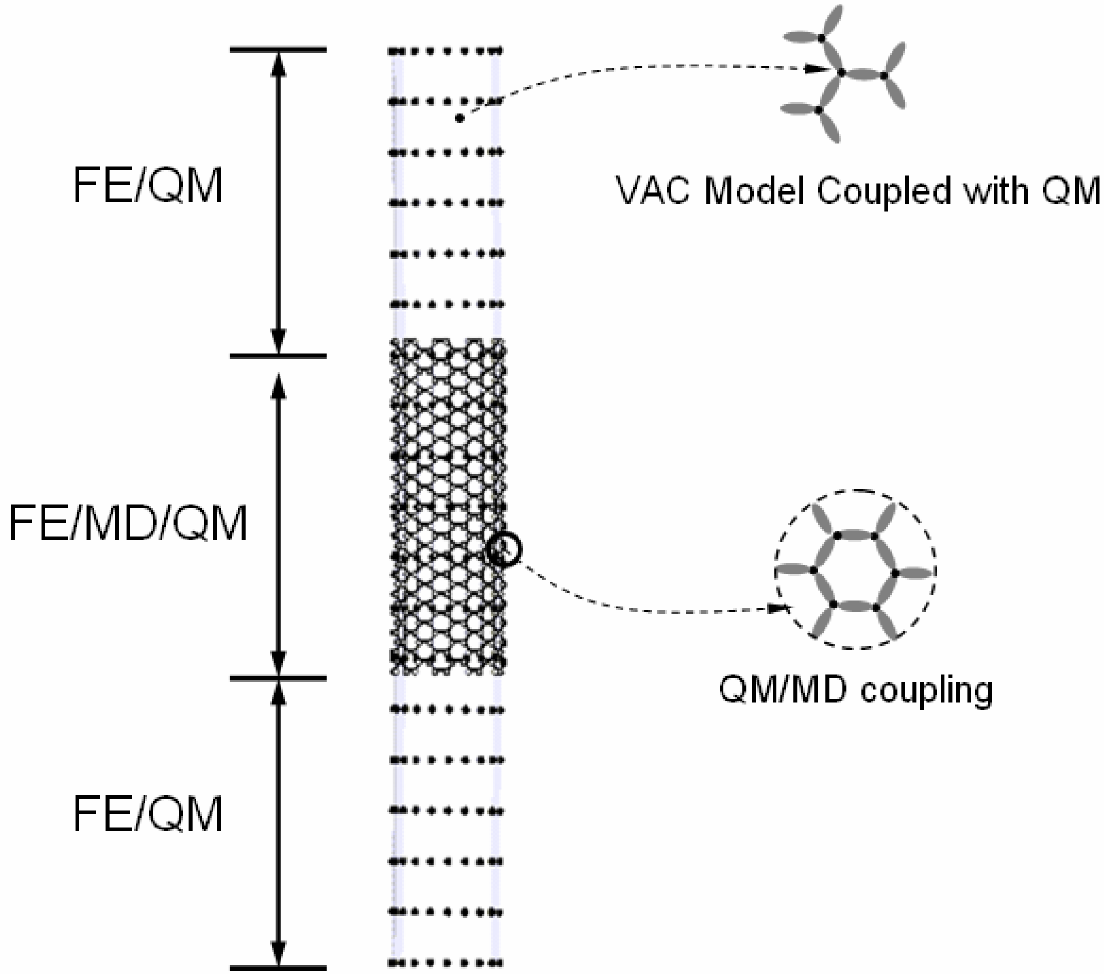
- Electronic aspect
  - The constitutive model to be built shall also include the information on the electrons
  - First principle calculations will be used to compute the electronic wave functions at a *local* scale corresponding to the constitutive model

Proposed Multiphysics Model: Embedding the Hierarchical Quantum-mechanical Model into Concurrent Scheme

- Finite elements/meshfree discretization defined in the entire domain as the "coarse scale" with the constitutive model based on first principle method

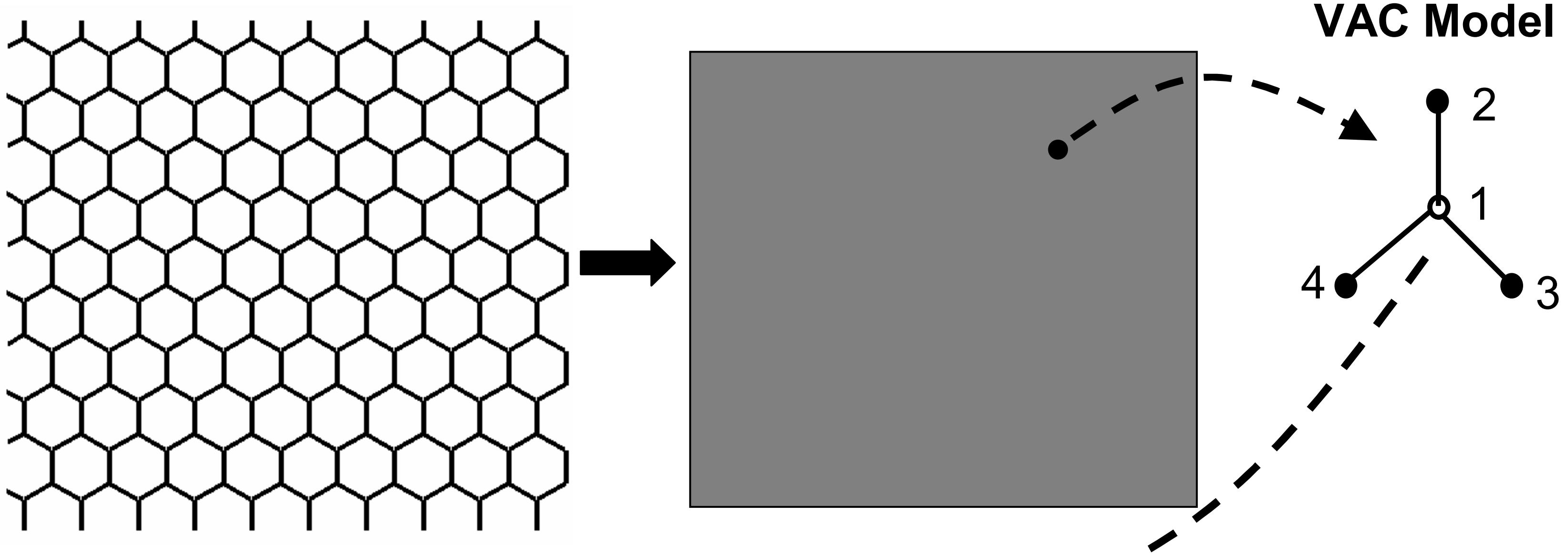
- In the fine scale region, FEM/Meshfree discretization co-exist with the molecular dynamics with potentials computed based on ab initio methods.

- Issues still being studied: time scale bringing, interface treatment……



Atomic Structure **Surface of distributed energy density**

VAC Model



$$W^{int}(\boldsymbol{u}) = \sum_{\alpha} \phi_{\alpha}(\boldsymbol{u}) = \int_{\Omega_0} \boxed{\phi_{\rho}(\boldsymbol{u})}\, d\Omega_0 \;\longrightarrow\; \delta W^{int}(\boldsymbol{u}) = \int_{\Omega_0} \frac{\partial \phi_{\rho}(\boldsymbol{u})}{\partial \boldsymbol{u}} \delta \boldsymbol{u}\, d\Omega_{\boldsymbol{0}}$$

For the graphite structure shown $\phi_{\rho}(\boldsymbol{u}) = \phi_{\rho}(\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3, \boldsymbol{u}_4)$

Coupling VAC model with quantum-mechanical method

- The advantage of the VAC model is that it directly depends on the atomic degree of freedom instead of any continuum measures.

- A fully coupled approach

$$\boxed{H|\psi\rangle = E|\psi\rangle} \Longleftrightarrow \boxed{m_\alpha \ddot{\boldsymbol{u}}_\alpha = -\frac{\partial E}{\partial \boldsymbol{r}_\alpha}} \Longleftrightarrow \boxed{\boldsymbol{N}^T \boldsymbol{f}_\alpha(\boldsymbol{u}) = \boldsymbol{N}^T m_\alpha \ddot{\boldsymbol{u}}_\alpha}$$

1. Quantum mechanical method solves the electronic wave functions ψ and the Energy states *E*. The spatial derivative of *E* gives the inter-atomic interactions

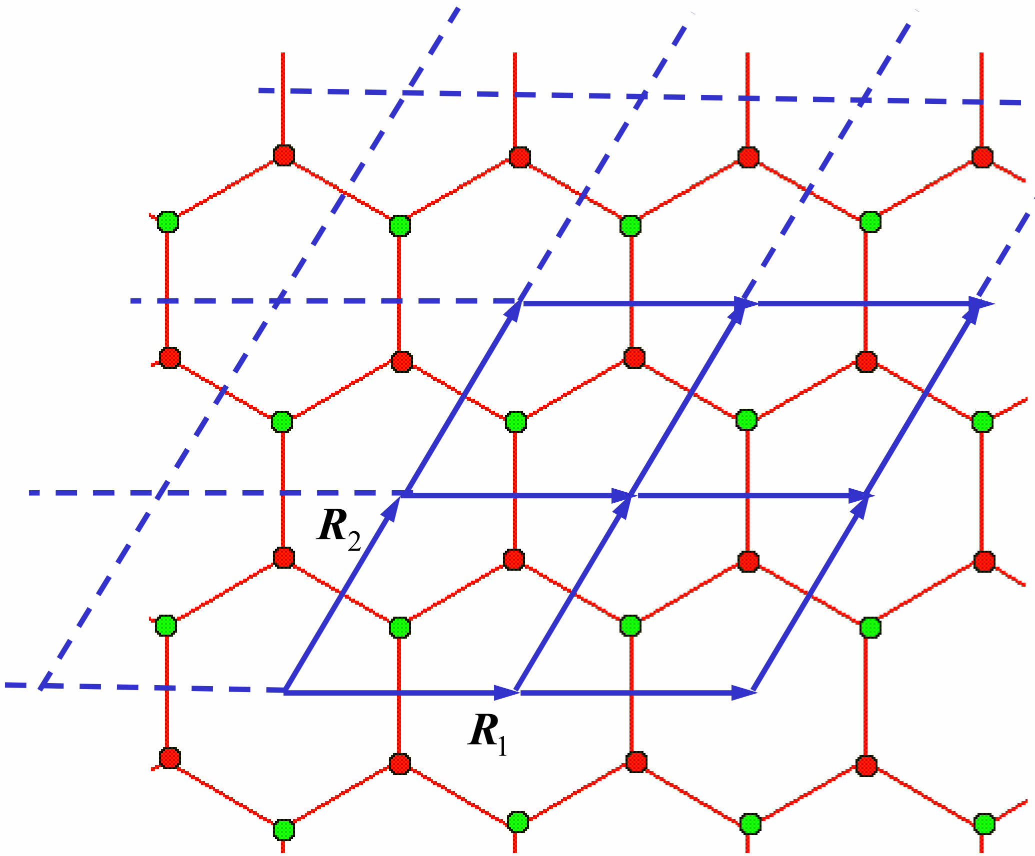
2. The VAC model solves the FEM equation based on the inter-atomic interactions. Provide the updated atomic position.

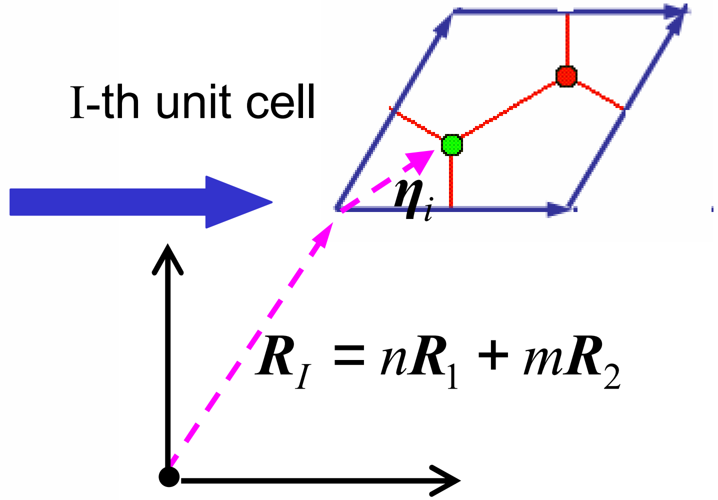
3. Based on the new atomic position, the Schrodinger equation is being solved for The next step.

4. The VAC model can be coupled with many quantum-mechanical approaches.

Coupling TB with VAC model in Carbon (sp2 Hybridization)

$$\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_I e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_I+\boldsymbol{\eta}_i)} \left|\varphi_\alpha(\boldsymbol{r}-\boldsymbol{R}_I\text{-}\boldsymbol{\eta}_i)\right\rangle$$





•The Linear combination of the base orbitals is given as

$$\left|\Psi(\boldsymbol{k},\boldsymbol{r})\right\rangle = \sum_{i\alpha} C_{i\alpha} \left|\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle$$

Coupling TB with VAC model in Carbon (sp2 Hybridization)

•The Schrödinger equation becomes

$$H\sum_{i\alpha} C_{i\alpha}\left|\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle = E\sum_{i\alpha} C_{i\alpha}\left|\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle$$

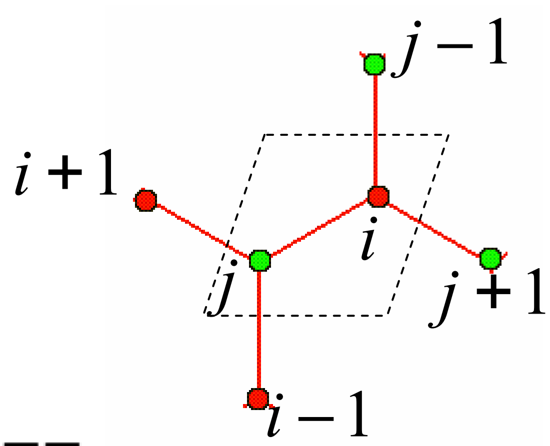
• Based on the variational principle used in TB approach, $C_{i\alpha}$ is solved from

$$\left|\boxed{\left\langle \psi_{j\beta}(\boldsymbol{k},\boldsymbol{r})\right|H\left|\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle} - E\boxed{\left\langle \psi_{j\beta}(\boldsymbol{k},\boldsymbol{r}) \middle| \psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle}\right| = 0$$

$$\left\langle \psi_{j\beta}(\boldsymbol{k},\boldsymbol{r})\right|H\left|\psi_{i\alpha}(\boldsymbol{k},\boldsymbol{r})\right\rangle = \sum_{L} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_L+\boldsymbol{\eta}_l)}\left\langle \varphi_\beta\left(\boldsymbol{r}-\boldsymbol{R}_J-\boldsymbol{\eta}_j\right)\right|H\left|\varphi_\alpha\left(\boldsymbol{r}-\boldsymbol{R}_I-\boldsymbol{\eta}_i\right)\right\rangle$$

with $\boldsymbol{R}_L = \boldsymbol{R}_J - \boldsymbol{R}_I$ $\quad \boldsymbol{\eta}_l = \boldsymbol{\eta}_j - \boldsymbol{\eta}_i$ $\quad \left\langle \varphi_\beta\left(\boldsymbol{r}-\boldsymbol{R}_J-\boldsymbol{\eta}_j\right) \middle| \varphi_\alpha\left(\boldsymbol{r}-\boldsymbol{R}_I-\boldsymbol{\eta}_i\right)\right\rangle = \delta_{\alpha\beta}\delta_{IJ}\delta_{ij}$

If only nearest neighbors are considered



	i-th atom	j-th atom
i-th atom	H_1	$\sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{d}_{ij}} H(\boldsymbol{d}_{ij})$
j-th atom	$\sum_i e^{i\boldsymbol{k}\cdot\boldsymbol{d}_{ji}} H(\boldsymbol{d}_{ji})$	H_1

8 × 8 matrix

Procedure to solve the TB-based VAC model

1. Based on interpolation using shape functions, prescribe deformed configuration of the unit cell with the coordinates of the atoms.

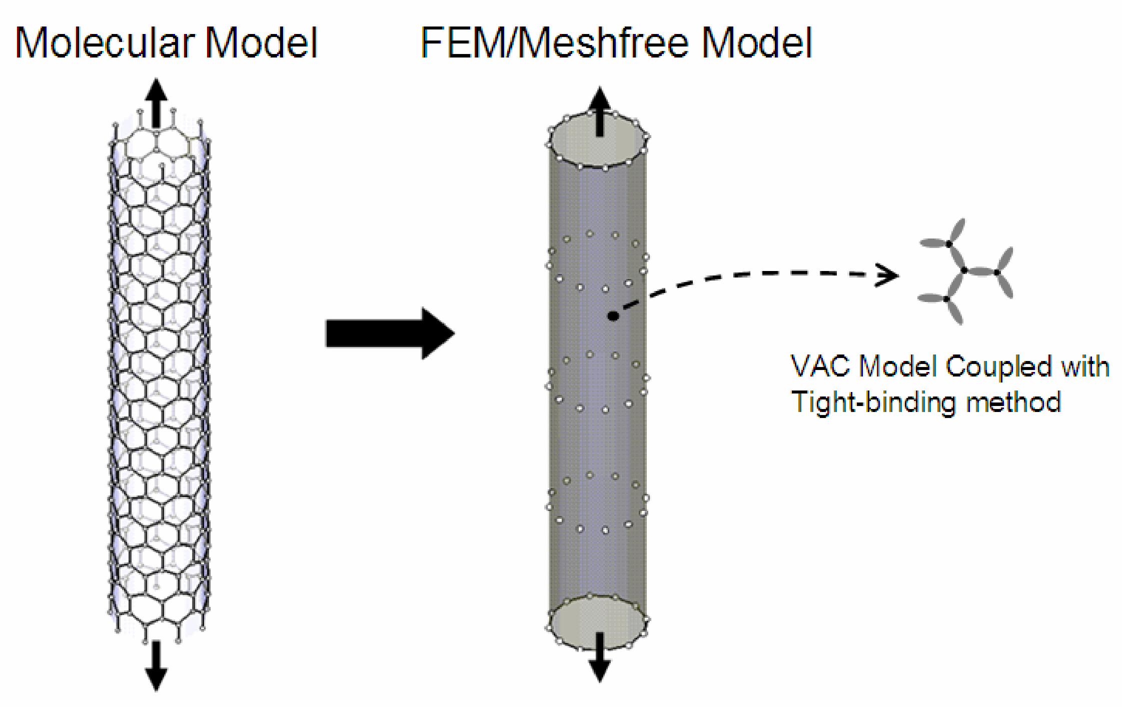
2. For wave vectors within the 1st Brillouin zone, evaluate the Hamiltonian matrix.

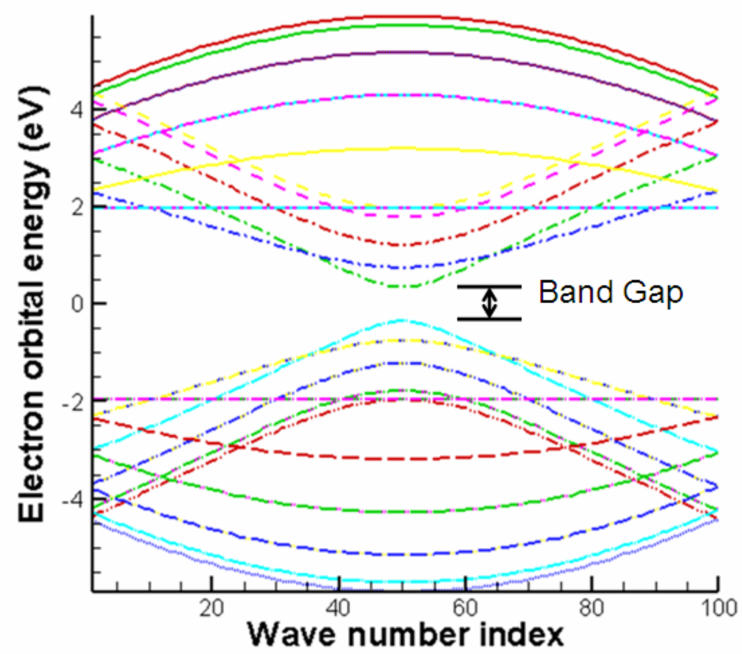
3. Solve eigen-value problem to obtain the energy level and electronic wave function.

4. Evaluate the bonding forces (Hellmann-Feynman theorem, Hellmann 1937, Feynman 1939)

$$f_{\alpha i}^{TB} = -\frac{\partial E^{TB}}{\partial x_{\alpha i}} = -\frac{\partial \langle \psi | H | \psi \rangle}{\partial x_{\alpha i}} = -\langle \psi | \frac{\partial H}{\partial x_{\alpha i}} | \psi \rangle$$

Preliminary Results: Tension/twisting of CNT

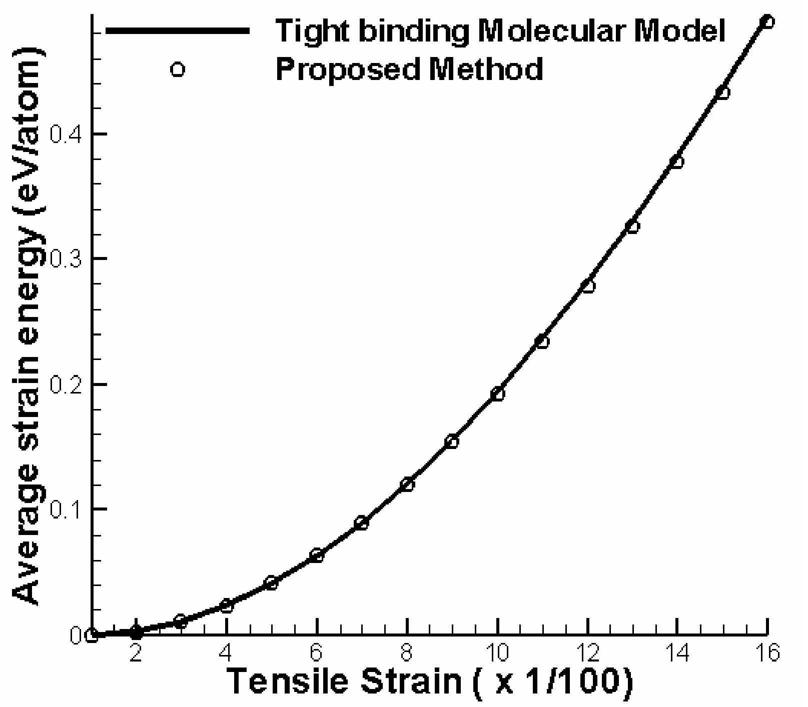


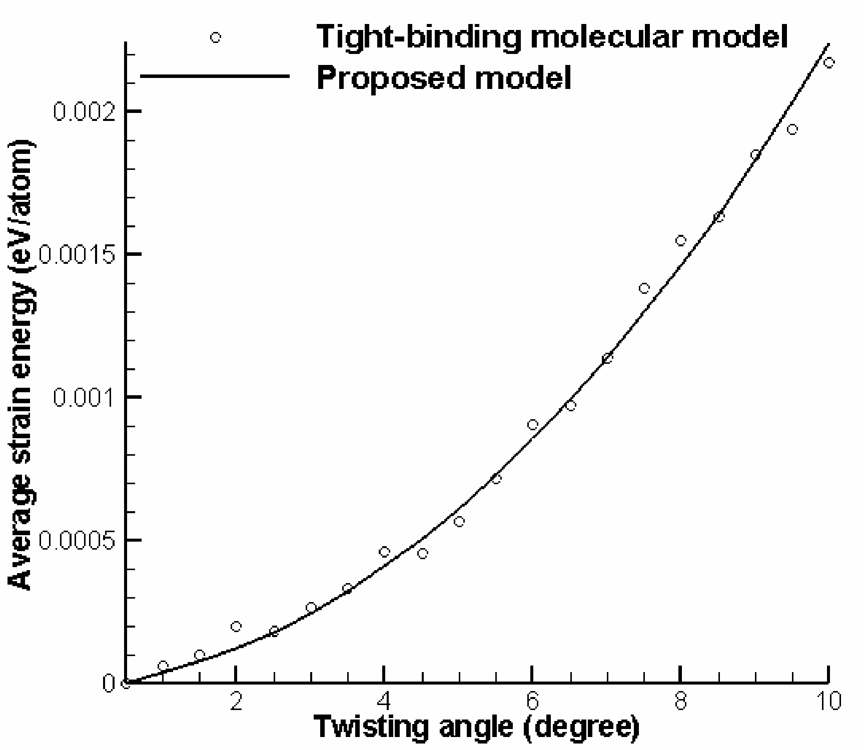


Molecular model: (9,0) CNT, 360 atoms
Coarse grain model: 60 computational particles
Loading condition: tension and twisting

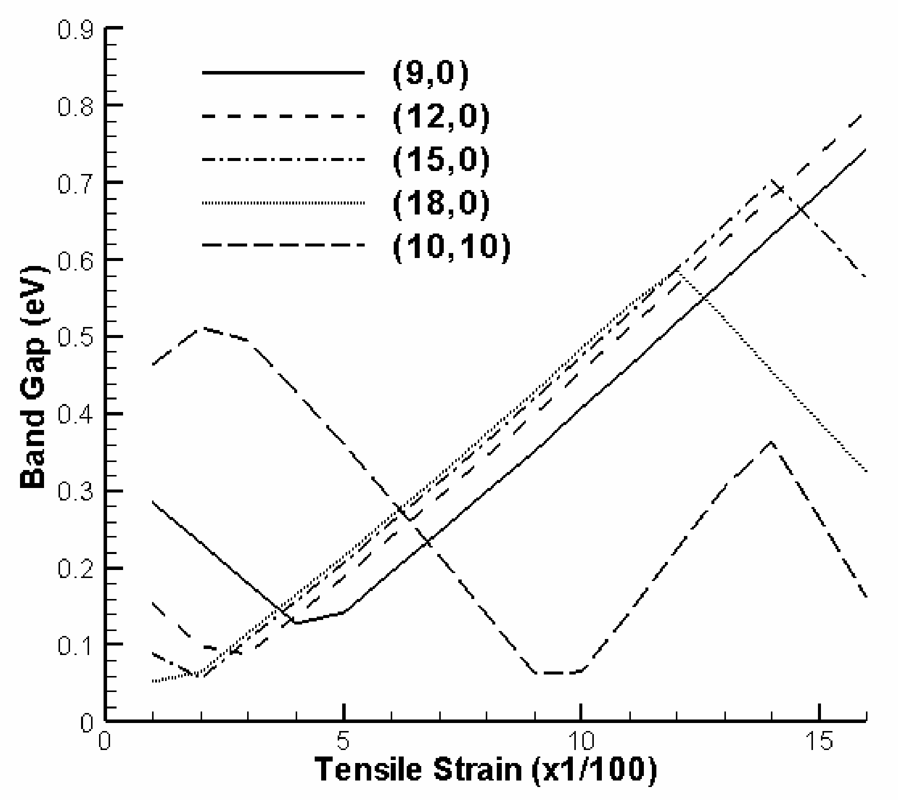
Electronic structure at zero strain

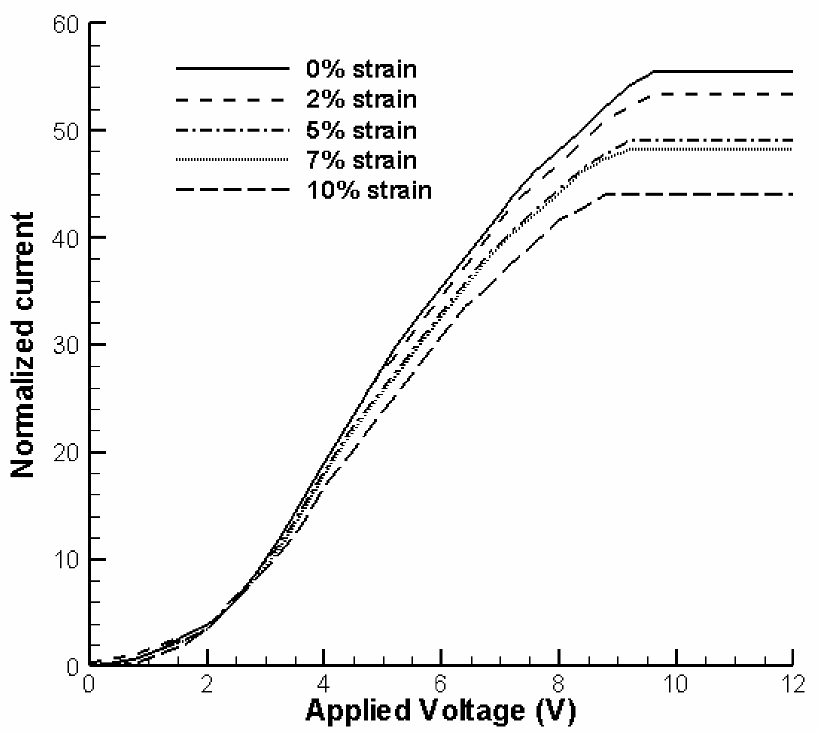
Comparison with Full-scale tight-binding Method





The Effect of Tensile Deformation on the Electronic Properties





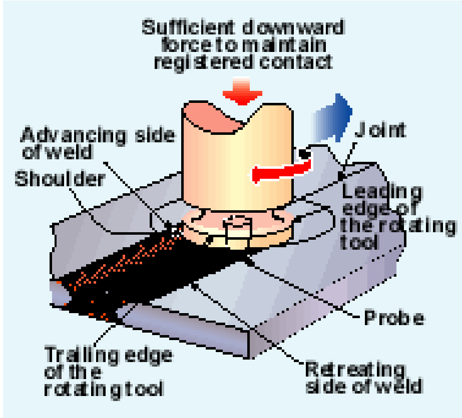
References

[1] Qian, D., Wagner, G.J., and Liu, W. K., (2004), A multiscale projection method for the analysis of carbon nanotubes, *Comput. Meth. Appl. Mech. Eng.* 193(17-20): 1603-1632.

[2] Qian, D. and Gondhalekar, R.H., (2004), A virtual atom cluster approach to the mechanics of nanostructures , *International Journal for multiscale computational engineering*. 2(2): 277-289.

[3] Liu, W.K., Sukky, J., and Qian, D., *Computational nanomechanics of materials (to appear)*, in *Handbook of theoretical and computational nanotechnology*, M. Reith and W. Schommers, Editors. 2006, American Scientific Publishers.

Friction Stir Welding: An example of the importance of microstructure when predicting fatigue and fracture:

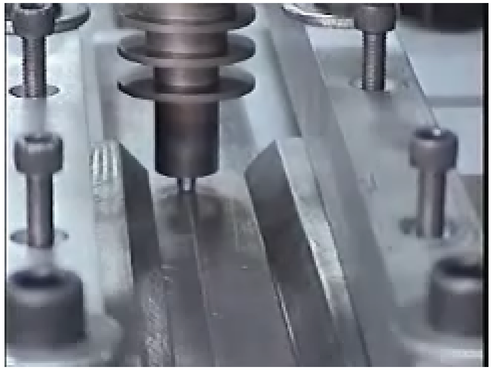


Friction stir welding rotary

http://www.twi.co.uk/j32k/unprotected/band_1/fswintro.html

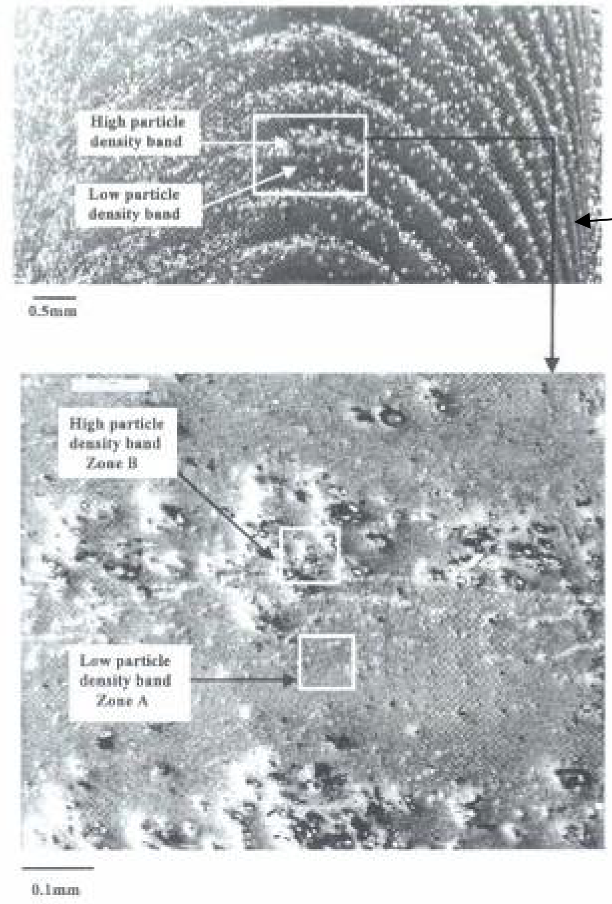
Complicated processing –microstructure relationship

- Rotating steel pin pierces a hole
- Rotating pin moves in direction of weld
- Friction heat aids severe plastic deformation - *NO MELTING OCCURS*
- Plasticized material driven to rear of pin
- Material consolidates, cools to form bond

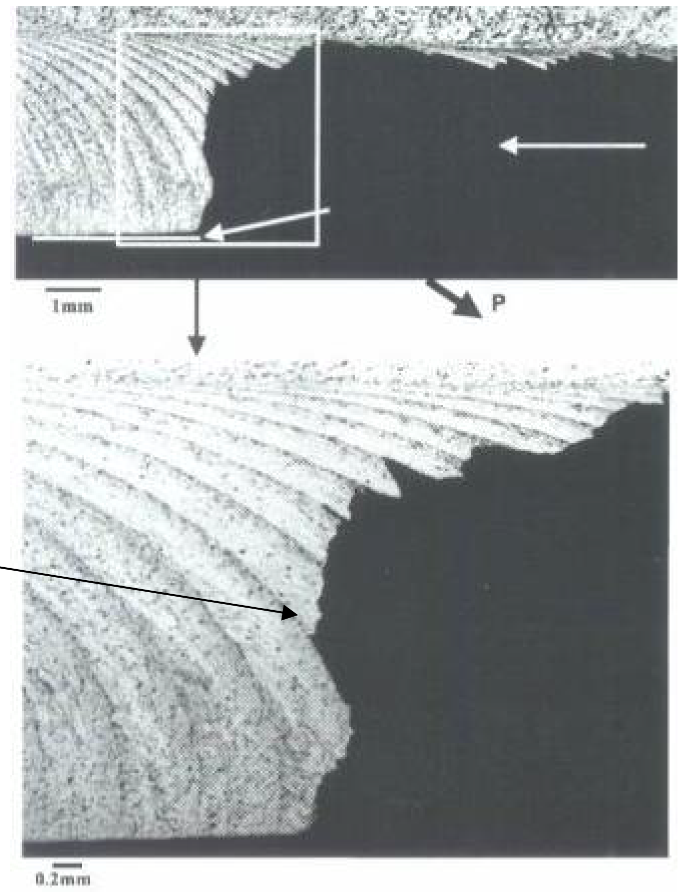


W.H. Paulo Martins Instituto Tecnico Superior

Motivation - Multiscale Continuum



Banded microstructure occurs during FSW process



Fracture occurs along regions of high particle density

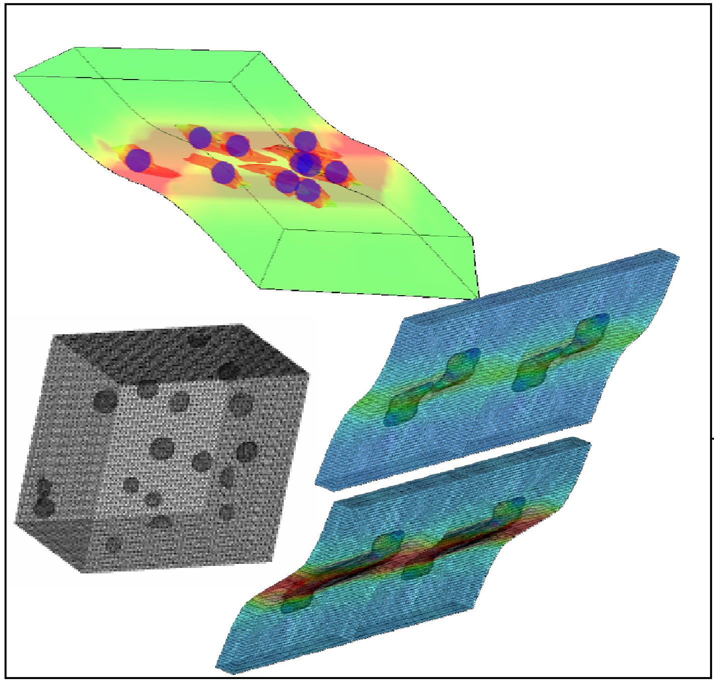
Hardness greater in high particle density bands due to greater Cu, Fe, Mg composition

Fracture can only be predicted if microstructural effects are included

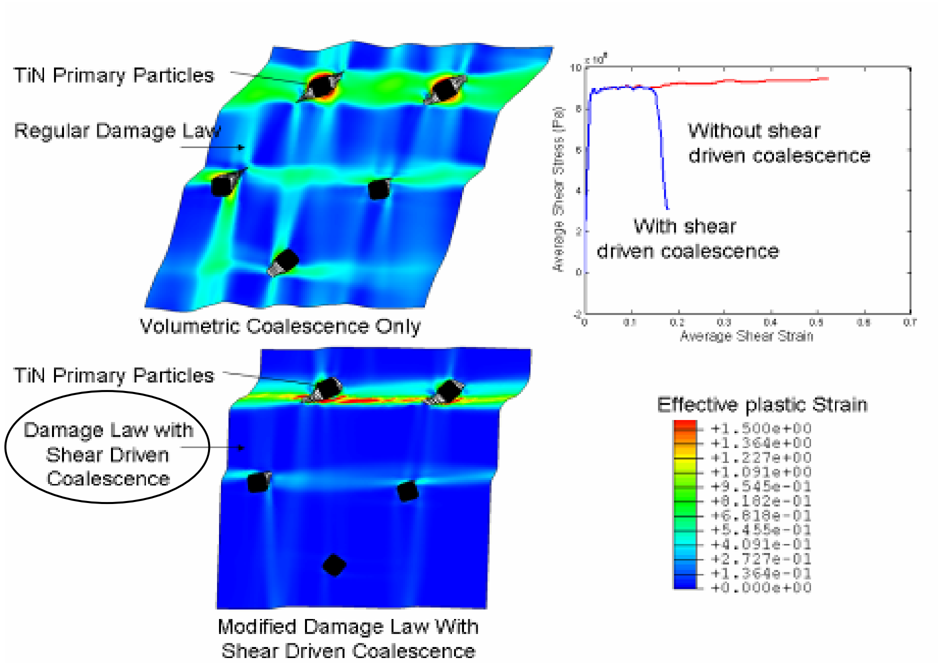
Conventional Approach e.g. Gurson (1977), Hao, Liu & Chang (2002), Internal State Variable (Bammann, Horstemeyer)

- Multiscale aspect introduced thru constitutive law
- Macroeffects (e.g. softening) function of microcauses (e.g. dislocation climb, glide, annihilation, damage, grain size effects)
- Micromechanics mathematically embedded in constitutive equations
- History effects captured e.g. Bausinger effect
- Standard governing equations are solved
- *Local* behavior only – No physical gradient effects are captured

TiC Particle Scale ~ 50 nm



TiN Particle Scale ~ 5 micron



McVeigh, Vernerey, Liu, Moran, Olson, "Identification and Modeling of a Microvoid Shear Localization Mechanism in High Strength Steels"

Concurrent Multiscale Continuum Theory

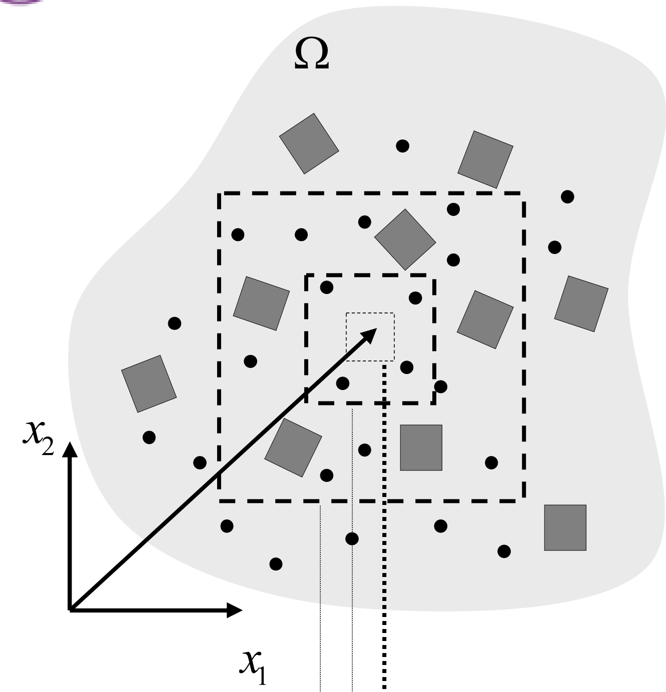
$$\delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F} + \sum_n \underbrace{\overline{\boldsymbol{\beta}}^n : \left(\delta\mathbf{F}^n - \delta\mathbf{F}\right) + \overline{\overline{\boldsymbol{\beta}}}^n \vdots \nabla\left(\delta\mathbf{F}^n\right)}$$

Non-local correction at scale *n*

- Extension of gradient theory to *n* scales
- Extra deformation fields describe the deformation at each scale
- Gradients at each scale
  - are preserved
  - and influence the total solution
- Mechanism based constitutive laws at each scale
- Physically: constitutive behavior depends on the length scale of localization

McVeigh, Vernerey, Liu, Brinson, “Multiresolution Analysis for Material Design” To appear in *Computer Methods in Applied Mechanics and Engineering*

Three Scale Decomposition of Steel



Governing equations

$$\begin{cases} \left(\boldsymbol{\sigma} - \bar{\boldsymbol{\beta}}^1 - \bar{\boldsymbol{\beta}}^2\right)\cdot\overleftarrow{\nabla} = 0 \\ \bar{\boldsymbol{\beta}}^1 - \bar{\bar{\boldsymbol{\beta}}}^1\cdot\overleftarrow{\nabla} = 0 \\ \bar{\boldsymbol{\beta}}^2 - \bar{\bar{\boldsymbol{\beta}}}^2\cdot\overleftarrow{\nabla} = 0 \end{cases}$$

Boundary conditions

$$\begin{cases} \left(\boldsymbol{\sigma} - \bar{\boldsymbol{\beta}}^1 - \bar{\boldsymbol{\beta}}^2\right)\cdot\mathbf{n} = \mathbf{t} \\ \bar{\bar{\boldsymbol{\beta}}}^1\cdot\mathbf{n} = 0 \\ \bar{\bar{\boldsymbol{\beta}}}^2\cdot\mathbf{n} = 0 \end{cases}$$

Constitutive equations

Three yield functions

$$\Phi\left(\boldsymbol{\sigma}\right)$$

$$\Phi^1\left(\bar{\boldsymbol{\beta}}^1, \bar{\bar{\boldsymbol{\beta}}}^1\right)$$

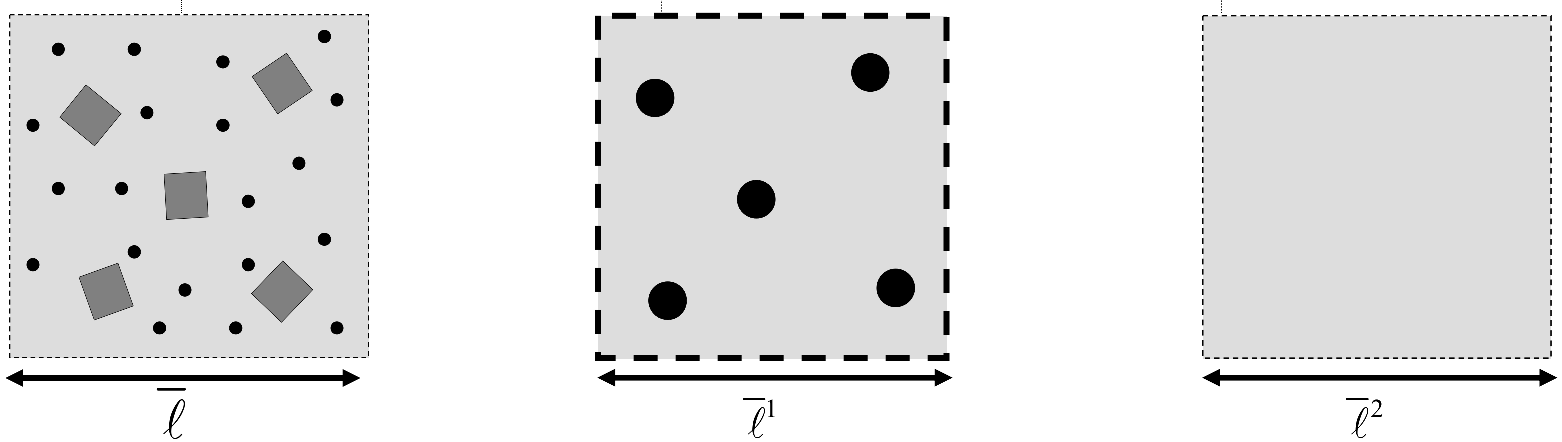
$$\Phi^2\left(\bar{\boldsymbol{\beta}}^2, \bar{\bar{\boldsymbol{\beta}}}^2\right)$$

Plastic strain increment

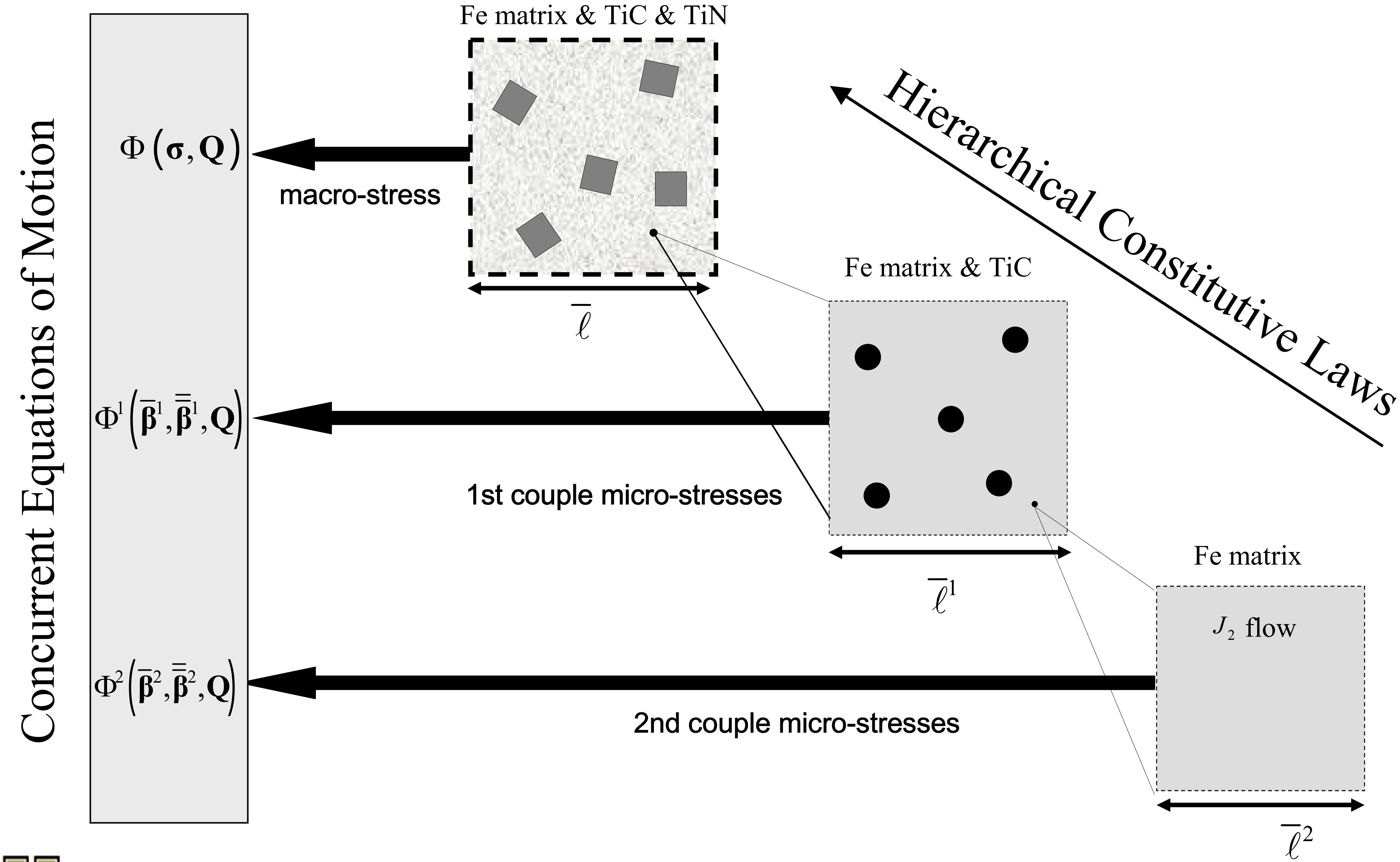
$$\mathbf{D}^p = \lambda\,\partial\Phi/\partial\boldsymbol{\sigma}$$

$$\left(\left(\mathbf{D}^1 - \mathbf{D}\right)^p, \mathbf{D}^{1p}\right) = \lambda^1\,\partial\Phi^1\Big/\partial\left(\bar{\boldsymbol{\beta}}^1, \bar{\bar{\boldsymbol{\beta}}}^1\right)$$

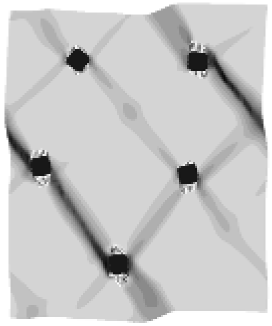
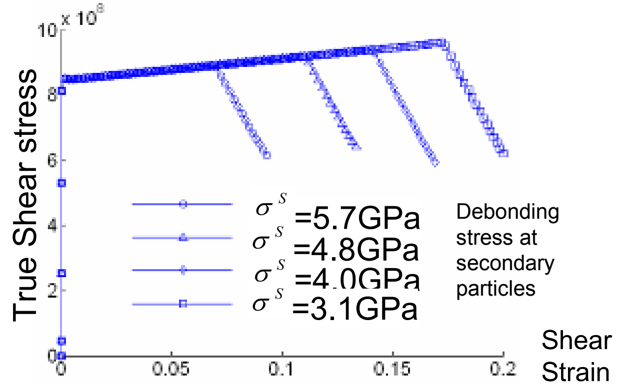
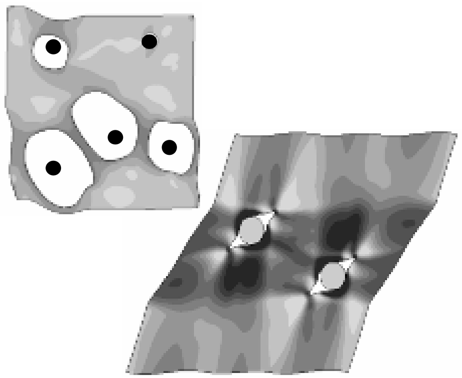
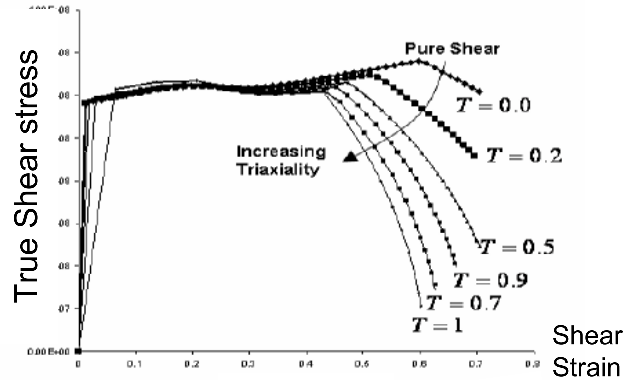
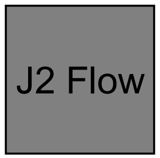
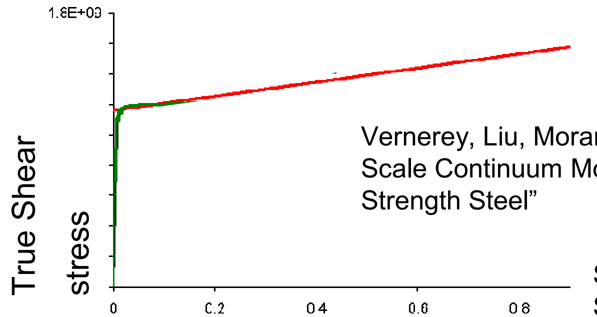
$$\left(\left(\mathbf{D}^2 - \mathbf{D}\right)^p, \mathbf{D}^{2p}\right) = \lambda^2\,\partial\Phi^2\Big/\partial\left(\bar{\boldsymbol{\beta}}^2, \bar{\bar{\boldsymbol{\beta}}}^2\right)$$



Derivation of the Constitutive Relation

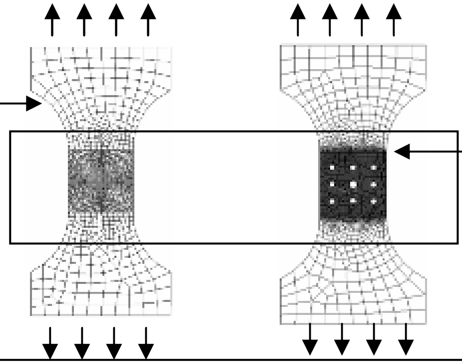


Summary of the Constitutive Relation

	Cell model	Plasticity model	Behavior in pure shear
Macro-scale		$\Phi(\boldsymbol{\sigma})$ Damage model (Gurson) with void sheet mechanism	
1st Micro-scale		$\Phi^1\left(\bar{\boldsymbol{\beta}}^1,\bar{\bar{\boldsymbol{\beta}}}^1\right)$ Damage model (Gurson) including shear softening	
2nd Micro-scale	 Softening after void coalescence 	$\Phi^2\left(\bar{\boldsymbol{\beta}}^2,\bar{\bar{\boldsymbol{\beta}}}^2\right)$ J2 flow plasticity	 Vernerey, Liu, Moran, “A Three Scale Continuum Model of High Strength Steel”

Two-scale porous material: Tensile specimen

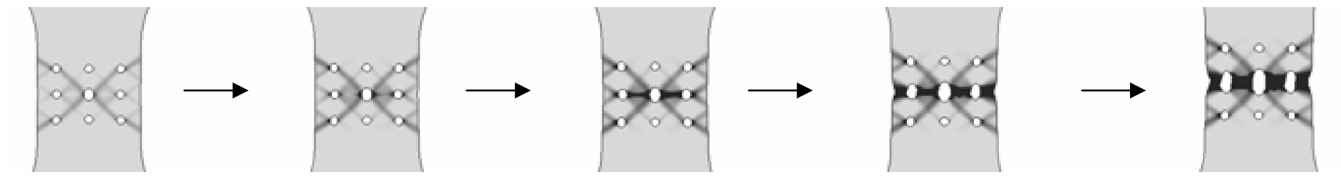
Two-scale
continuum mesh



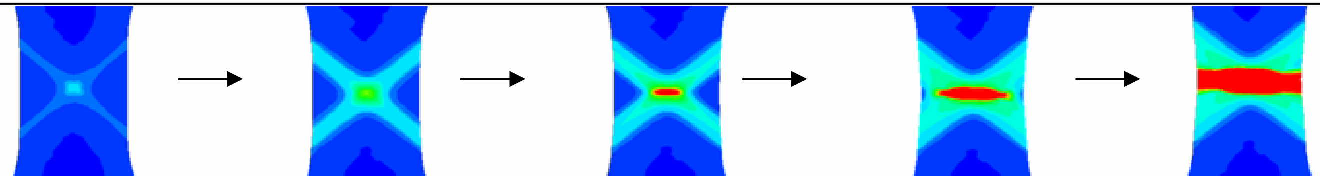
Explicit microstructure
mesh

VERNEREY, LIU, MORAN
(Northwestern University)

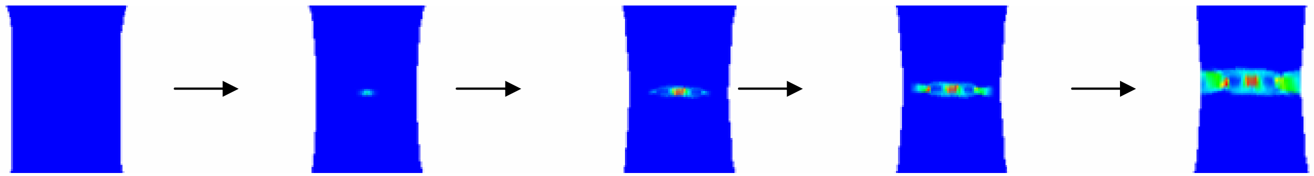
Explicit microstructure



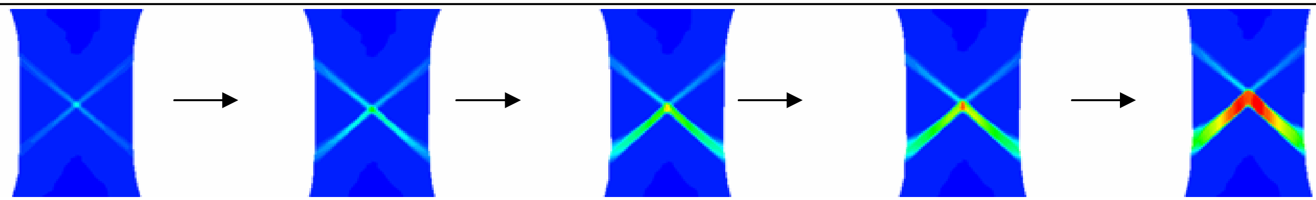
Two-scale continuum
Plastic macro-strain



Two-scale continuum
Void coalescence

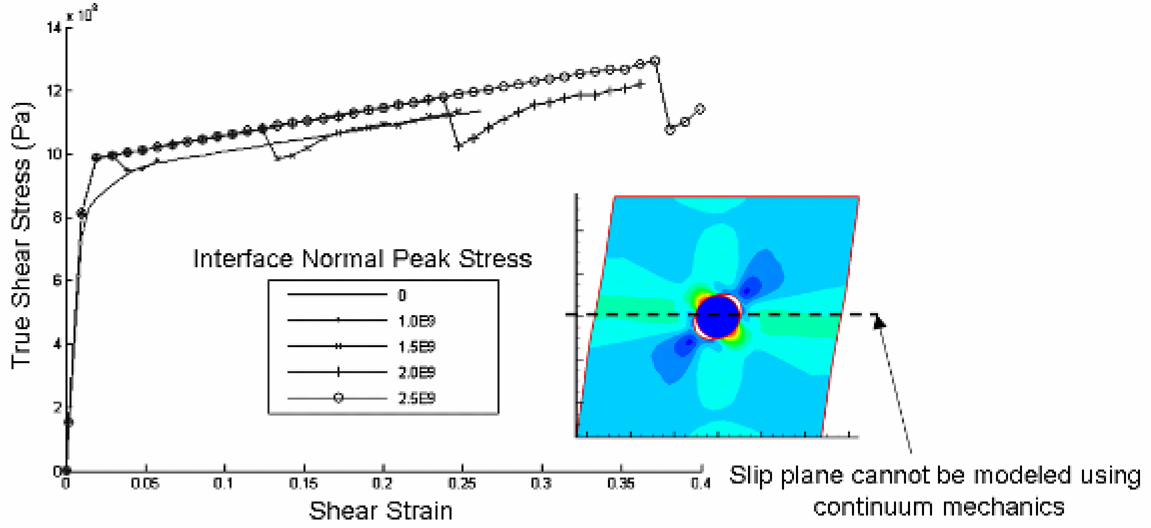


Conventional continuum
Plastic strain



Many problems are too large for the Bridging scale (Atomic-Continuum Coupling) Method and too small to be examine using a multiscale continuum method

E.g. post debonding softening due to micro-particle decohesion



Build up of elastic energy which unloads into slip plane

Bridging Continuum and Discrete Multiscale Theory

- Multi-physics & multi-resolution theory
  - *Bridge between discrete atomic scale theory and multiscale continuum theory*
- Smooth transition between continuum fields and discrete atomic behavior
  - *Virtual representation of the atomic lattice*
- Simple adaptive scheme to identify where the solution needs further refinement
  - *Criterion arises naturally in multiresolution analysis*

Displacement Field at *n*th nested scale

$$\tilde{\mathbf{u}}^n(\mathbf{X}) = \sum_{\mathrm{I}} \underbrace{\mathrm{N}_{\mathrm{I}}^n(\mathbf{X})}_{\text{Mapping Function, scale } n} \mathbf{u}(\mathbf{X}_{\mathrm{I}}^n) \qquad n = 1 \ldots N$$

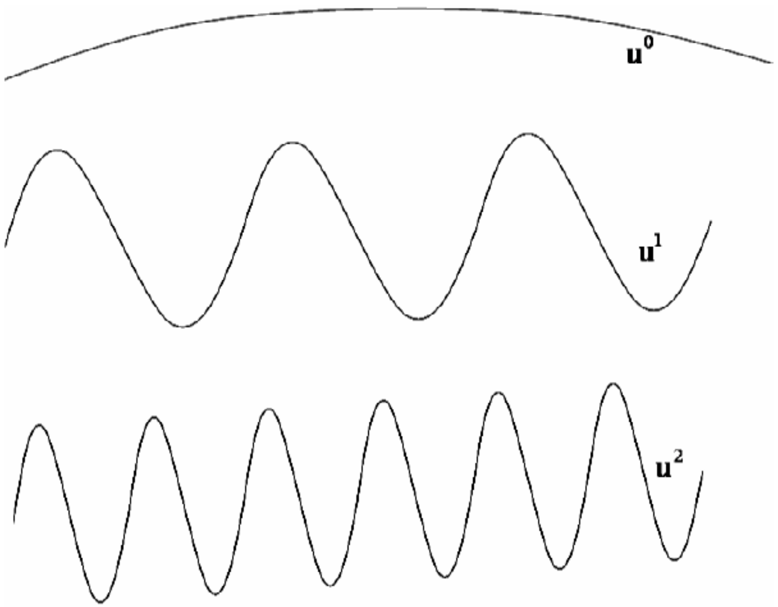
The relative displacement:

$$\mathbf{u}^n(\mathbf{X}) = \tilde{\mathbf{u}}^n(\mathbf{X}) \qquad n = 0$$

$$\mathbf{u}^n(\mathbf{X}) = \tilde{\mathbf{u}}^n(\mathbf{X}) - \tilde{\mathbf{u}}^{n-1}(\mathbf{X}) \qquad n = 1 \ldots N$$

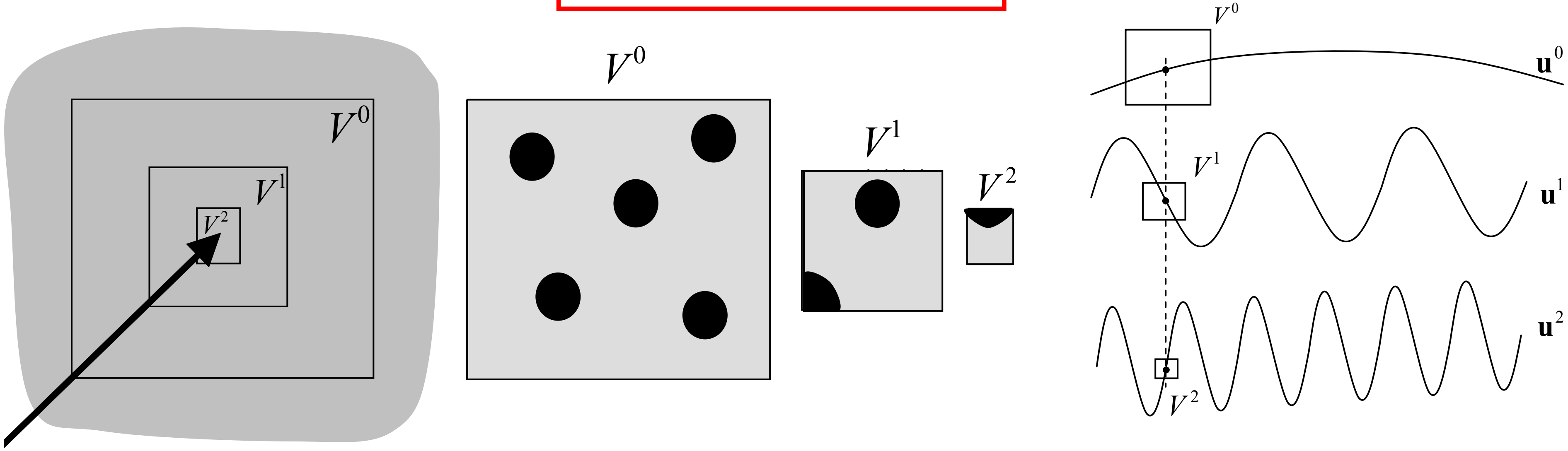
Approximation converges to the real solution:

$$\tilde{\mathbf{u}}^N = \sum_{n=1}^{N} \mathbf{u}^n \quad \text{where } \tilde{\mathbf{u}}^N \to \mathbf{u} \text{ as } N \to \infty$$



- Multiresolution internal work density is decomposed to each scale *n*: $\boxed{\delta\tilde{w}_{\text{int}}^{N} = \sum_{n=0}^{N} \mathbf{f}^{n} \bullet \delta\mathbf{u}^{n}}$

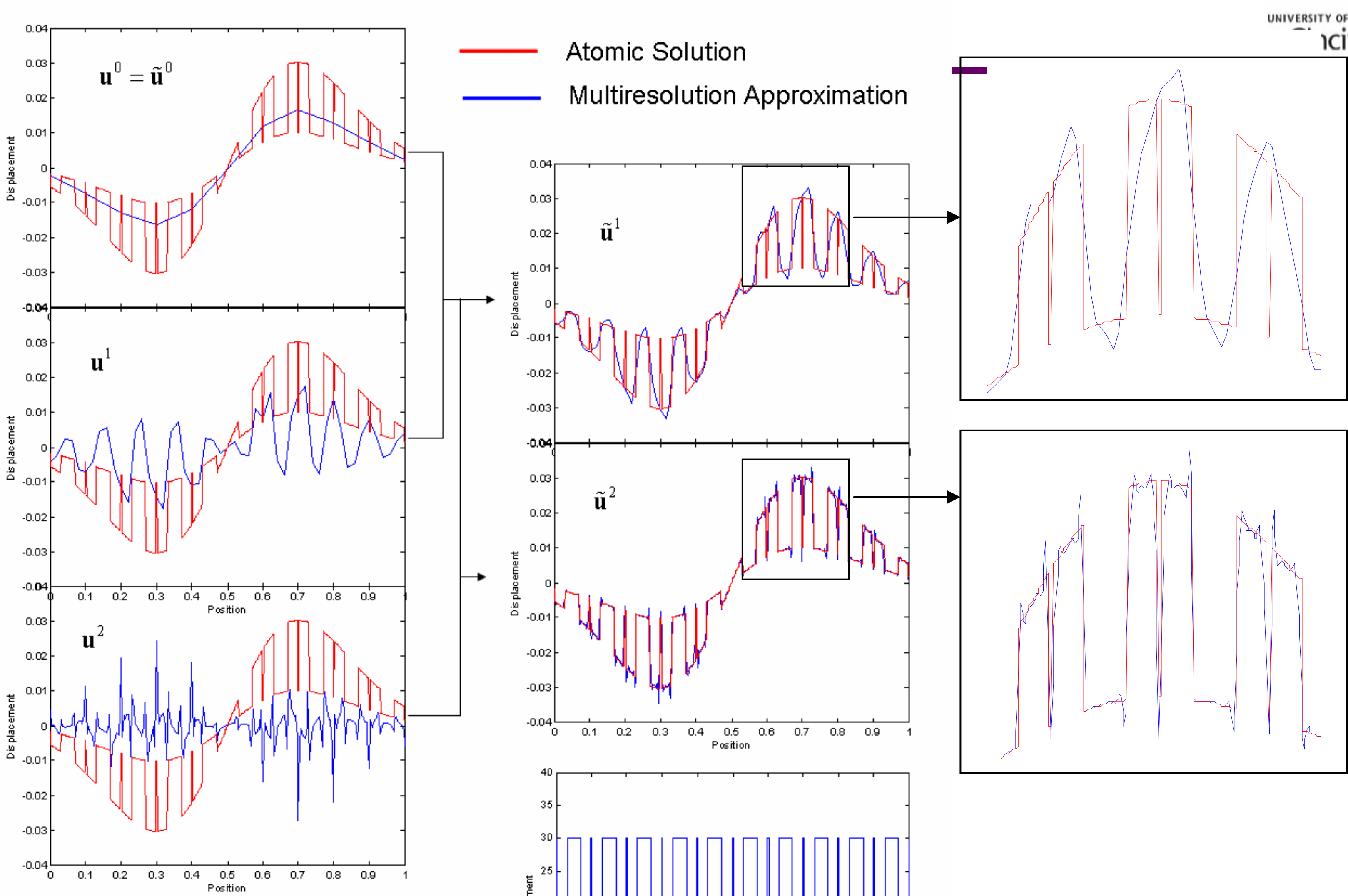
- An N scale VAC approach: $\boxed{\delta\tilde{w}_{\text{int}}^{N} = \sum_{n=0}^{N} \left(\sum_{\alpha=1}^{\alpha^{n}} \mathbf{f}_{\alpha}^{n} \bullet \delta\mathbf{u}_{\alpha}^{n} \right)}$

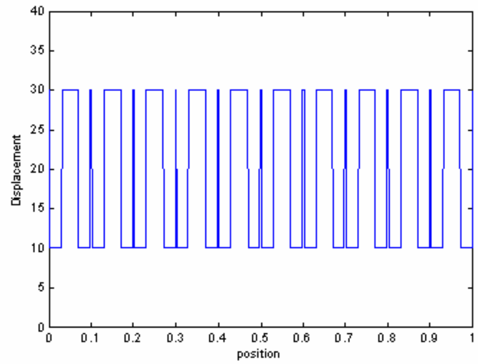


- Averaging volume at each scale defines the constitutive behavior – using VAC the constitutive behavior at each scale in computed 'on the fly'

Summation → Integral

- At larger scales, the averaging volume size is much larger: $\boxed{\delta\tilde{w}_{\text{int}}^{N} = \sum_{n=0}^{N} \left(\frac{1}{V^{n}} \int_{V^{n}} \mathbf{f}^{n} \bullet \delta\mathbf{u}^{n} dV^{n} \right)}$





Microstructure with two characteristic length scales

Scale One captures large particles, scale two captures small particles

Multiscale Continuum - Discrete

• Multiresolution theory formulated consistently with the Multiscale continuum theory

• Multiscale couple stress is replaced by the relative force arising between scales

• Challenge is to have a seamless transition between:

Multiscale continuum theory → Multiresolution theory

Gradient effects thru non-local averaging

Gradient effects thru strain gradient

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